PENTAGONAL BIPYRAMIDAL COMPLEXES OF FIRST-ROW TRANSITION METALS

By

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KEY TO ABBREVIATIONS

PB	pentagonal bipyramidal
CFSE	crystal field stabilization energy
EDTA	ethylenediaminetetraacetate
DAP	2,6-diacetylpyridine
SCA	semicarbazide hydrochloride
PH	2-pyridylhydrazine
DAPSC	2,6-diacetylpyridinebissemicarbazone
DAPP	2,6-diacetylpyridinebis-2-pyridylhydrazone
NMR	nuclear magnetic resonance
IR	infrared
UV	ultraviolet
Vis	visible
ASCACHOPY	2-acetylsemicarbazone-6-acetyl-3-hydroxopyridine

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PENTAGONAL BIPYRAMIDAL COMPLEXES OF FIRST-ROW TRANSITION METALS

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Major Department: Chemistry

The synthesis and study of complexes with potentially planar pentadentate Schiff base ligands were undertaken. Template reactions or direct combination of a metal salt and a ligand were used to prepare pentagonal bipyramidal (PB) complexes of the elements Mn through Zn. X-ray structural studies were carried out to confirm the coordination geometry and to investigate the factors influencing seven-coordination.

The structures were solved by locating the metal atoms in Patterson functions and remaining atoms in Fourier syntheses. The trial structures were refined by least-squares techniques. For isomorphous structures, the coordinates from one structure were used as a starting set for the others.

The isomorphous series of complexes of Mn(II), Fe(II), Co(II), and Zn(II) with 2,6-diacetylpyridinebissemicarbazone

forms monoclinic crystals, space group I_a. These are the first reported PB complexes of Fe(II), Co(II), and Zn(II). The average metal-donor distances in the pentagonal plane follow the trend of ionic radii, but the metal-axial water and metal-axial chloride distances decrease on going from Mn(II) to Zn(II). Steric and electronic factors related to this decrease are discussed.

Dichloro-2,6-diacetylpyridinebissemicarbazoneiron(III) chloride dihydrate forms red monoclinic needles, space group $P2_{1/c}$. The PB complex has average distances of 2.200(2) for Fe-N, 2.10(3) for Fe-O, and 2.34(2)Å for Fe-Cℓ. Bond lengths in the Fe(II) and Fe(III) complexes are compared.

Air oxidation of a solution of copper(II) chloride, 2,6-diacetylpyridine, and semicarbazide hydrochloride yields chloroaqua(2-acetylsemicarbazone-6-acetyl-3-hydroxopyridine) copper(II) as monoclinic green plates, space group $C_{2/c}$. The complex is square pyramidal with typical metal-ligand distances.

Diaqua-2,6-diacetylpyridinebissemicarbazonenickel(II) nitrate and the isomorphous Mn(II) complex form monoclinic crystals, space group $P2_{1/n}$. The isostructural Cu(II) complex forms yellow monoclinic plates, space group $P_{2/m}$. These are the first reported PB complexes of Ni(II) and Cu(II). The metal-ligand distances follow the trends observed earlier in this work. Factors influencing the planarity of the ligand are discussed.

Diaqua-2,6-diacetylpyridinebis-2-pyridylhydrazonecobalt

(II) chloride and the isomorphous Zn(II) complex form monoclinic crystals, space group $P2_{1/n}$. The complexes have PB geometry. The average metal-ligand distances are in agreement with the trends followed by the PB complexes described above. The steric interactions between terminal pyridine rings are discussed.

The dimeric complex 2,6-diacetylpyridinebis-2-pyridylhydrazonozinc forms red monoclinic plates, space group $C_{2/c}$. The coordination geometry is distorted octahedral. The first reported bridging pyridine nitrogen-zinc distances are 2.39(1) and 2.59(1)Å. The remaining Zn-N distances average 2.041(8)Å. Factors influencing the twisting of the ligand are discussed.

The crystal field stabilization energies for PB and octahedral complexes are compared. The role of ligand constraints in producing PB complexes is discussed. The structural results are related to d orbital splittings. Complexes with 2,6-diacetylpyridinebis-2-pyridylhydrazone are compared to earlier work.

INTRODUCTION

Seven-coordinate first-row transition metal complexes cannot be considered at all common. Among the factors believed to contribute to the relative instability of these species are increased ligand-ligand repulsion, weaker bonds, and reduced crystal field stabilization energy as a result of nonoctahedral geometry.[1] Examples of possible geometries include the pentagonal bipyramid (PB); the capped octahedron, in which a seventh ligand has been added to one of the eight triangular faces; and the capped trigonal prism, in which a seventh ligand has been added to the rectangular face of the trigonal prism.

At the start of this work, very few seven-coordinated structures of first-row metals had been determined. Those which were known were largely with ions of d^5 or d^{10} electronic structure, where the lack of crystal field stabilization energy (CFSE) results in no favored geometry. Some structures contained bidentate ligands with small bites, such as nitrate and oxalate. The seven-coordinate Mn(II) and Fe(III) complexes of EDTA contain a coordinated water molecule in addition to the hexadentate ligand.[2,3] The geometries of these complexes do not conform to any regular shape. Two Fe(III) complexes with the Schiff base ligand formed from 2,6-diacetylpyridine and triethylenetetramine have PB structures.[4] Two bidentate nitrate ions in the complex $Zn(py)_3(NO_3)_2$ produce a seven-coordinate structure of irregular geometry.[5] Several peroxochromate anions have been shown to have PB structures.[6] An approximate PB configuration exists about the titanium atoms of μ-oxalatobis(oxalato)hexa-aquodititanium(III)tetrahydrate.[7]

During the course of this work several heptacoordinate complexes were characterized. Chlorotris(N,N-dimethyldithiocarbamato)titanium(IV) contains discreet seven-coordinate molecules which have a somewhat distorted PB structure,[8,9] and tris(N,N-diethyldithiocarbamato)oxo-vanadium(V) contains PB geometry about the vanadium atoms.[10] The heptacyanovanadate(III) anion[11,12] represents the sole example of a seven-coordinate complex of a first-row transition metal containing seven identical ligands. The geometry is only slightly distorted from perfect D_{5h} symmetry. Trinitrato-2,2'-bipyridylmanganese(III) contains two bidentate nitrate ions and the resulting complex has irregular PB configuration.[13] The recently determined structure[14] of a macrocyclic complex of Mn(II) contains an "unusually regular" PB coordination polyhedron.

In order to systematically study the properties of PB complexes of first-row transition metals, the design of ligands which would consistently produce PB complexes was necessary. Transition metal complexes of Schiff base ligands are well known, and the subject has been reviewed.[15,16] Several methods of preparation of these complexes, among which is the very useful template reaction, have been described.[17,18] Many of the resulting complexes contain macrocyclic ligands, and excellent reviews on this topic are available.[19-22]

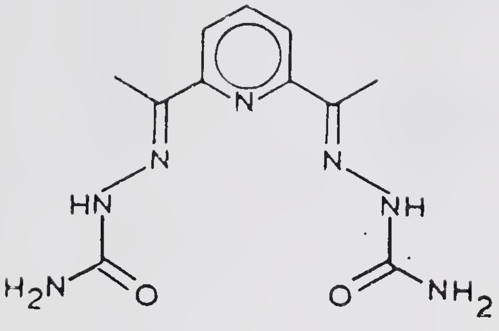
Several ligands derived from 2,6-diacetylpyridine (DAP) and various amines through condensation and formation of Schiff bases appeared reasonably well suited to our needs. Some of these ligands are depicted in Figure 1. Such ligands are particularly interesting since the backbone should be fairly rigid due to the conjugation present. Therefore, the probability of producing complexes containing planar pentadentate ligands is increased. If monodentate ligands coordinate above and below the plane of the ligand, the resulting complex has PB configuration. Many of the ligands in Figure 1 have ionizable protons and in most cases dinegative ligands should be readily produced. The complexes of these anionic chelates were predicted to be pentagonal planar due to the conjugation in the ligand backbone.[23] Therefore, a study of the complexes formed with the above pentadentate ligands was undertaken.

FIGURE 1

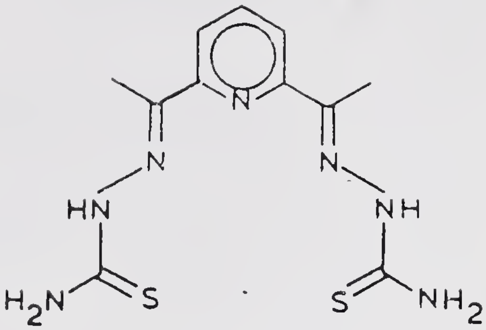
POTENTIAL PLANAR PENTADENTATE LIGANDS

Schiff base ligands are formed by condensation of DAP with (a) SCA, (b) thiosemicarbazide, (c) PH, (d) 2-picolylamine, (e) o-aminobenzenethiol, (f) o-phenylenediamine, (g) triethylenetetramine, and (h) tetrahydrofurfurylamine.

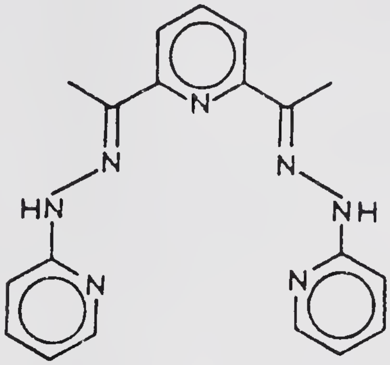
(a) is DAPSC, (c) is DAPPH.



(a)



(b)



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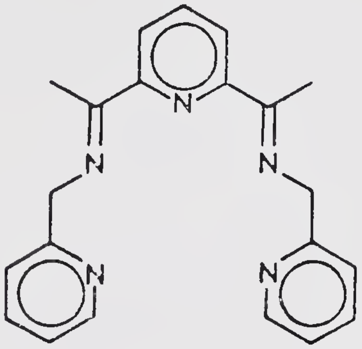
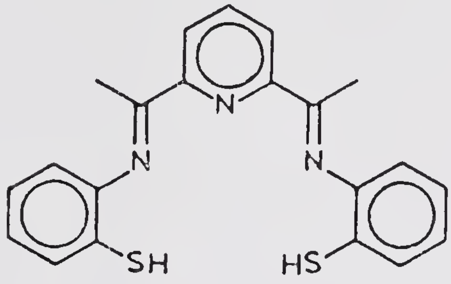
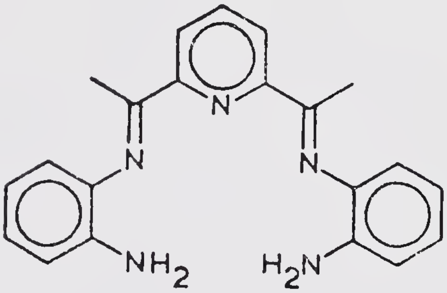


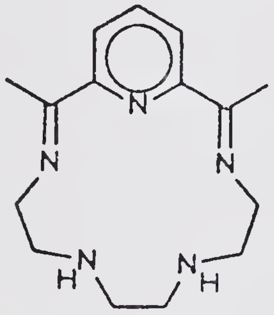
(d)



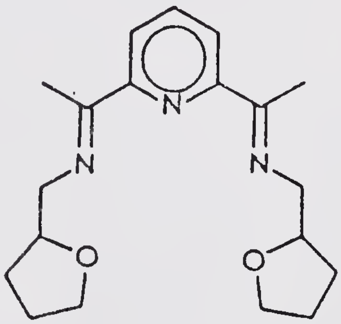
(e)



(f)



(g)



(h)

GENERAL DIFFRACTION EXPERIMENTAL

The following is a general description of the experimental method used in the structure solutions. The method is applicable to all solutions except where explicitly noted in the text.

Precession and Weissenberg photographic[24,25] data were used to calculate the preliminary space group and cell constants. Least-squares fittings of 2Θ, Ω, X, and Φ for fifteen intense reflections centered on a Syntex $P\bar{1}$ diffractometer gave accurate cell constants with standard deviations and the orientation matrix for data collection. The unit cell volume and its standard deviation were determined from the cell constants. The calculated density was generally in agreement with the density measured by the flotation method.[26] The density of the solvent was measured to ±0.01 $\frac{g}{cc}$ with a precision hygrometer.

The suitability of a crystal for data collection was determined by its physical shape, the ease with which reflections were centered, and the value of the accurate cell constants and their estimated standard deviations. All intensity measurements were made at ambient temperature with a Syntex $P\bar{1}$ diffractometer. All unique reflections up to a limiting 2Θ value were measured using a variable speed Θ-2Θ scan technique. The scan rate was determined from a three-second intensity measurement of the reflection and varied linearly from 1°/minute for counts of 150.0 or less to 24°/minute for 1500.0 counts or more. The intensity, I, was equal to:

$$I = \text{scan rate}\left[\text{total scan counts} - \frac{(\text{background counts})}{(\text{background to scan ratio})}\right]$$

Peaks were scanned from 1° below $K\alpha_1$ to 1° above $K\alpha_2$. Background counts were taken at each end of the range. The estimated standard deviation, $\sigma(I)$, of each reflection is given by:

$$\sigma(I) = \left[\text{total scan counts} + \frac{(\text{background count})^2}{(\text{background to scan ratio})}\right]^{\frac{1}{2}}$$

The incident beam was monochromatized by a low order reflection of graphite for molybdenum radiation and by 0.35 mil nickel foil for copper radiation. Any changes in the system were detected by measuring four standard reflections after each 96 intensity measurements.

A standardized data set was obtained by scaling the data to the initial value of the sum of the standard reflections. Any duplicate or equivalent reflections were averaged. Reflections with intensity greater than $K\sigma(I)$, where K is given in Table 1, were considered observed. The unobserved reflections were deleted from further steps in the structure solution and were identified by a minus sign. Corrections for Lorentz-Polarization of the form:

$$^{1}/_{LP} = {}^{\sin 2\Theta}/_{(1+\cos^2 2\Theta)}$$

and for assuming the monochromator of Mo radiation to be 50% perfect crystal and 50% mosaic were applied where appropriate. Scattering factors were obtained from Hanson, Herman, Lea, and Skillman;[27] Stewart, Davidson, and Simpson;[28] Doyle and Turner;[29] and are uncorrected for anomalous dispersion. The natural log of the scale factor and the overall temperature factor were estimated from a Wilson plot.[30] The initial choice of a centric or acentric space group was made on the basis of calculated intensity statistics.[31]

The heavy atom or atoms were located using a Patterson function[32] of the form:

$$P(UVW) = \frac{2}{V} \sum_{h=0}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} |F(hkl)|^2 \cos 2\Pi(hU+kV+lW)$$

The heavy atom approximation allowed the phase of each reflection, $\alpha(hkl)$, to be determined. The determination of other atomic positions was possible through use of Fourier syntheses[32] of the form:

$$P(XYZ) = \frac{2}{V} \sum_{h=0}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} |F(hkl)| \cos 2\Pi[(hX+kY+lZ)-\alpha(hkl)].$$

The atoms located in each Fourier synthesis were used as a starting set for the next calculation. This process was repeated until all non-hydrogen atom positions were located.

The trial structure was refined by least-squares minimization[32] of the function:

$$\text{Residual} = \Sigma w(\,\big||Fobs| - |Fcalc|\big|\,)^2,$$

where:

$$\sqrt{w} = {}^{Fobs}/_{A} \quad \text{for } Fobs < A$$

$$\sqrt{w} = 1.0 \quad \text{for } A \le Fobs \le B$$

$$\sqrt{w} = {}^{B}/_{Fobs} \quad \text{for } Fobs > B,$$

and A and B are constants given in Table 1. Prior to refinement an overall scale factor was chosen such that the sum of

F_{obs} equaled the sum of F_{calc}. Initially isotropic and then anisotropic temperature factors of the form:

$$\exp\left[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + \beta_{12}hk + \beta_{13}hl + \beta_{23}kl)\right]$$

were used. R, the reliability index, is given by:

$$R = \frac{\Sigma \left| |Fobs| - |Fcalc| \right|}{\Sigma |Fobs|}$$

Calculations were performed on IBM $^{360}/_{65}$ and $^{370}/_{165}$ computers with programs written or modified by Dr. G. J. Palenik.

Table 1
CRYSTALLOGRAPHIC DATA

COMP.	CRYSTAL CLASS	SYSTEMATIC ABSENCES	SPACE GROUP (s)	CRYSTAL SIZE
[Mn(DAPSC)(H_2O)Cl]Cl·$2H_2O$	monoclinic	hkl, h+k+l=odd h0l, h=odd	Ia, $I_{2/a}$	0.19x0.27x0.29 mm.
[Fe(DAPSC)(H_2O)Cl]Cl·$2H_2O$	"	"	"	0.07x0.24x0.28
[Co(DAPSC)(H_2O)Cl]Cl·$2H_2O$	"	"	"	0.09x0.09x0.18
[Zn(DAPSC)(H_2O)Cl]Cl·$2H_2O$	"	"	"	0.20x0.23x0.26
[Fe(DAPSC)Cl_2]Cl·$2H_2O$	"	h0l, l=odd 0k0, k=odd	$P_{2_1/c}$	0.10x0.10x0.25
Cu(H_2O)(ASCACHOPY)Cl·½H_2O	"	hkl, h+k=odd h0l, l=odd	C_c, $C_{2/c}$	0.15x0.37x0.38
[Mn(DAPSC)(H_2O)$_2$](NO_3)$_2$·H_2O	"	h0l, h+l=odd 0k0, k=odd	$P_{2_1/n}$	0.37x0.35x0.06
[Ni(DAPSC)(H_2O)$_2$](NO_3)$_2$·H_2O	"	"	"	0.07x0.35x0.42
[Cu(DAPSC)(H_2O)$_2$](NO_3)$_2$·H_2O	"	h0l, l=odd	P_c, $P_{2/c}$	0.35x0.44x0.48
[Co(DAPSC)(H_2O)$_2$]Cl_2	"	h0l, h+l=odd 0k0, k=odd	$P_{2_1/n}$	0.16x0.19x0.33
[Zn(DAPPH)(H_2O)$_2$]Cl_2	"	"	"	0.13x0.20x0.25
Zn(DAPP)·$CHCl_3$·H_2O	"	hkl, h+k=odd 0k0, k=odd	C_c, $C_{2/c}$	0.11x0.11x0.16

Table 1 - extended

ABS. COEFF.	RAD. USED	a	b	c	β	VOLUME
10.4 cm^{-1}	Mo	18.322(3)Å	13.076(5)Å	8.128(1)Å	99.98(1)°	1917.9(8)Å^3
11.4	Mo	18.096(2)	13.111(4)	8.061(1)	99.76(1)	1884.8(6)
12.8	Mo	17.968(3)	13.139(8)	8.052(2)	99.86(2)	1872.9(13)
13.5	Cu	18.038(11)	13.112(5)	8.066(3)	100.28(4)	1877.1(6)
12.2	Mo	12.317(1)	12.960(2)	14.225(2)	119.82(1)	1970.0(5)
18.5	Cu	16.568(3)	11.062(4)	15.096(4)	91.03(2)	2766.2(13)
7.6	Mo	11.489(3)	14.964(4)	12.359(6)	105.55(3)	2047.0(12)
10.5	Mo	11.493(2)	14.914(4)	12.154(4)	104.94(2)	2012.8(9)
11.8	Mo	10.977(4)	13.930(3)	6.977(3)	104.55(3)	1032.6(6)
10.9	Mo	8.004(3)	27.373(11)	10.341(2)	105.39(2)	2184.5(12)
14.3	Mo	7.887(2)	27.751(6)	10.377(3)	105.23(2)	2191.5(9)
14.3	Cu	18.842(7)	11.072(5)	22.893(5)	94.93(3)	4758 (3)

Table 1 - extended

ρ_c	ρ_o	2θ range	k(kσ)	#meas. refl.	#obs. refl.	R	A	B
1.584g/cc	1.59g/cc	0-35°	2.00	1271	1200	0.039	8.0	32.0
1.615	1.62	0-50	2.00	1675	1565	0.040	6.0	24.0
1.636	1.63	0-50	1.50	1671	1524	0.039	6.0	24.0
1.655	1.63	0-110	1.50	1186	1177	0.058	6.0	24.0
1.604	1.61	0-45	1.80	2594	2204	0.048	8.5	65.0
1.735	1.70	0-110	1.50	1749	1590	0.039	15.0	30.0
1.656	1.65	0-45	2.00	2704	1772	0.062	20.0	60.0
1.697	1.70	0-45	2.00	2646	1624	0.055	20.0	80.0
1.669	1.65	0-50	2.00	1826	1683	0.056	20.0	60.0
1.555	1.55	0-50	2.00	3378	2815	0.046	8.0	32.0
1.570	1.57	0-45	2.00	2889	2249	0.040	8.0	32.0
1.525	1.48	0-100	2.00	2364	1578	0.080	12.0	47.0

CHAPTER 3
SYNTHESIS AND CHARACTERIZATION

All reactions were carried out in air except where noted otherwise. DAPPH was stored in a desiccator. All solvents were reagent grade and were used without further purification. DAP was purchased from Aldrich Chemical Co., Inc., Milwaukee, Wis. and Pfaltz and Bauer, Inc., Flushing, N. Y. and was recrystallized from an ethanol-water mixture before use. Other chemicals and their suppliers are 2-pyridylhydrazine (PH), Aldrich; semicarbazide hydrochloride (SCA), $CoCl_2 \cdot 6H_2O$, 50% $Mn(NO_3)_2$ solution, and $CuCl_2 \cdot 2H_2O$, Fisher Scientific Co., Fair Lawn, N. Y.; $MnCl_2 \cdot 4H_2O$, $Ni(NO_3)_2 \cdot 6H_2O$, and $ZnCl_2$, Mallinckrodt Chemical Works, St. Louis, Mo.; $FeCl_3 \cdot 6H_2O$, $NiCl_2 \cdot 6H_2O$, Matheson, Coleman, and Bell, Norwood, Ohio; and $Co(NO_3)_2 \cdot 6H_2O$ and $Cu(NO_3)_2 \cdot 3H_2O$, J. J. Baker Chemical Co., Phillipsburg, N. J.

Infrared spectra were recorded on a Perkin-Elmer Model 337 Grating Infrared Spectrophotometer as KBr discs. Polystyrene film served as calibrant. Ultraviolet spectra were recorded using a Cary Model 14 recording spectrophotometer. Visible spectra were recorded on a Beckman DBG spectrometer.

Magnetic moments were calculated[33,34] from data obtained on a Varian A-60A Analytical NMR Spectrometer and from gram susceptibilities measured with a Varian Associates electromagnet using mercuric tetrathiocyanotocobaltate(II)[35] as a calibrant. Melting points were taken on a Mel-temp apparatus in open capillaries and are uncorrected. Microanalyses were performed by Galbraith Laboratories, Inc., Knoxville, Tenn.

2,6-Diacetylpyridinebissemicarbazone (DAPSC). To DAP (1.9537 g, 11.97 mmole) dissolved in 95% ETOH (100 ml) were added SCA (2.6700 g, 23.94 mmole) and sodium acetate (1.9638 g, 23.94 mmole). The mixture was stirred and water added until all solids dissolved. After ca. 1 min. a fluffy white precipitate formed. The precipitate was collected by filtration and washed with dilute ethanolic sodium hydroxide. Yield 2.70 g, 81%, m.p. 275°C.

2,6-Diacetylpyridinebis-2-pyridylhydrazone (DAPPH). PH (7.2 g, 66 mmole) and DAP (5.4 g, 33 mmole) were dissolved in 95% ETOH (100 ml) and stirred at reflux for 5 min. The yellow residue remaining after evaporation of solvent was recrystallized from abs. ETOH and stored in a desiccator. Yield 9.8 g, 84%.

$[\mathrm{Mn(DAPSC)(H_2O)Cl]Cl\cdot 2H_2O}$. To $\mathrm{MnCl_2\cdot 4H_2O}$ (0.4948 g, 2.5 mmole) dissolved in water (50 ml) was added SCA (0.5576 g, 5.0 mmole). To the resulting clear colorless solution was added DAP (0.4080 g, 2.5 mmole). The mixture was stirred and heated, becoming clear yellow upon complete solution of the DAP. Upon cooling a light yellow crystalline precipitate began forming. The precipitate was collected by filtration. Yield 0.97 g, 85%, m.p. 335-6°C.

$[\mathrm{Fe(DAPSC)(H_2O)Cl]Cl\cdot 2H_2O}$ and $[\mathrm{Fe(DAPSC)Cl_2]Cl\cdot 2H_2O}$. To $\mathrm{FeCl_3\cdot 6H_2O}$ (0.675 g, 2.5 mmole) dissolved in water was added

DAP (0.4080 g, 2.5 mmole). The DAP dissolved upon heating and SCA (0.5576 g, 5.0 mmole) was added to the warm orange solution. The color changed to deep red. The solution was left at room temperature for 24 hours, after which greenish-black crystals ($[Fe(DAPSC)(H_2O)Cl]Cl\cdot 2H_2O$) were formed. These were collected by filtration. Yield 0.26 g, 23% (based on Fe), m.p. >360°C. The filtrate was left at room temperature for two days, after which red needlelike crystals ($[Fe(DAPSC)Cl_2]Cl\cdot 2H_2O$) were formed. These were collected by filtration. Yield 0.53 g, 45%, m.p. >360°C. Reddish-black platelike crystals formed in the mother liquor after several days. Structural studies of these crystals have begun.

$\underline{[M(DAPSC)(H_2O)Cl]Cl\cdot 2H_2O \quad (M=Co,Zn)}$. To $CoCl_2\cdot 6H_2O$ (3.5690 g, 15 mmole) and DAP (2.4477 g, 15 mmole) in aqueous ethanol (33%, 150 ml) was added SCA (3.3456 g, 30 mmole) in water (50 ml). The red solution was stirred and solvent evaporated slowly. Red crystals formed overnight and were collected by filtration. Yield 3.8951 g, 56%, m.p. 336°C. In a similar manner colorless crystals of $[Zn(DAPSC)(H_2O)Cl]Cl\cdot 2H_2O$ were prepared using $ZnCl_2$. Yield 4.1575 g, 59%, m.p. 267°C.

$\underline{DAPSC\cdot NiCl_2\cdot 4H_2O}$. This complex was prepared in the same manner as $[Co(DAPSC)(H_2O)Cl]Cl\cdot 2H_2O$, using $NiCl_2\cdot 6H_2O$. Yield 4.2853 g, 60%, m.p. 320°C, green crystals.

$\underline{Cu(H_2O)(ASCACHOPY)Cl\cdot \frac{1}{2}H_2O \text{ and } DAPSC\cdot CuCl_2\cdot 2H_2O}$. To $CuCl_2\cdot 2H_2O$ (0.4262 g, 2.5 mmole) in water (50 ml) was added DAP (0.4080 g, 2.5 mmole). The DAP dissolved upon heating and SCA (0.5576 g, 5.0 mmole) was added to the warm blue-green solution. After a momentary deep blue color, the solution changed to dark green and then greenish-yellow. The solution was left overnight at room temperature after which dark green crystals ($Cu(H_2O)(ASCACHOPY)Cl\cdot\frac{1}{2}H_2O$) were formed. These were collected by filtration. Upon further evaporation of solvent, yellow crystals ($DAPSC\cdot CuCl_2\cdot 2H_2O$) formed and were collected by filtration.

In another experiment, $CuCl_2\cdot 2H_2O$ (2.5573 g, 15 mmole) and DAP (2.4477 g, 15 mmole) were dissolved in aqueous ETOH (33%, 150 ml) with N_2 bubbling through the solution. SCA (3.3459 g, 30 mmole) in water (50 ml) was added to the blue-green solution producing a transient deep blue color followed by a gradual change to greenish-yellow. Slow evaporation of solvent under N_2 produced yellow crystals ($DAPSC\cdot CuCl_2\cdot 2H_2O$). Yield 4.2706 g, 64%, m.p. 203°C.

$\underline{[M(DAPSC)(H_2O)_2](NO_3)_2\cdot H_2O\quad (M=Ni,Mn,Co,Cu)}$. To a slurry of DAPSC (0.6932 g, 2.5 mmole) in 95% ETOH (20 ml) was added a solution of $Ni(NO_3)_2\cdot 6H_2O$ (0.7270 g, 2.5 mmole) and concentrated HNO_3 (0.5 ml) in aqueous ethanol (50%, 40 ml). Mild heating produced a clear greenish-yellow solution and greenish-yellow crystals formed upon cooling and slow evaporation of solvent. Yield 0.86 g, 67%, m.p. 267°C. In a similar manner were prepared yellow crystals of $[Mn(DAPSC)(H_2O)_2](NO_3)_2\cdot H_2O$ (0.95 g, 74%, m.p. >360°C) using $Mn(NO_3)_2$ solution, orange crystals of $[Co(DAPSC)(H_2O)_2](NO_3)_2\cdot H_2O$ (0.82 g, 64%, m.p. 328°C) using $Co(NO_3)_2\cdot 6H_2O$, and yellow crystals of [Cu(DAPSC)$(H_2O)_2$]$(NO_3)_2 \cdot H_2O$ (0.79 g, 61%, m.p. 243°C) using $Cu(NO_3)_2 \cdot 3H_2O$.

[Co(DAPPH)$(H_2O)_2$]Cl_2. To a warm solution of DAPPH (0.8860 g, 2.5 mmole) in 95% ETOH (35 ml) was added a solution of $CoCl_2 \cdot 6H_2O$ (0.5948 g, 2.5 mmole) in 95% ETOH (25 ml). Concentrated HCl (0.5 ml) was added and the resulting deep reddish-brown solution was boiled, cooled and filtered. Slow evaporation of solvent produced red crystals ([Co(DAPPH)$(H_2O)_2$]Cl_2). Yield 0.58 g, 45%, m.p. >360°C.

[Zn(DAPPH)$(H_2O)_2$]Cl_2. This complex was prepared in the same manner as [Co(DAPPH)$(H_2O)_2$]Cl_2, using methanol-water (9:1) as solvent and $ZnCl_2$. Yield 0.63 g, 49%, m.p. 230°C, yellow crystals.

Zn(DAPP)$\cdot CHCl_3 \cdot H_2O$. To a warm solution of DAPPH (0.8860 g, 2.5 mmole) in acetone (50 ml) was added dropwise a slurry of $ZnCl_2$ (0.3407 g, 2.5 mmole) in acetone (25 ml). A reddish-orange precipitate formed. A solution of KOH (>0.28 g) in water (>50 Ml) was added dropwise producing a red solution and a black precipitate. The mixture was extracted with three portions of chloroform. The extracts were combined and dried over anhydrous $MgSO_4$. Slow evaporation of solvent in air produced red crystals. Yield 0.49 g, 36%, m.p.>360°C.

Results and Discussion

Synthesis. The most interesting feature of the syntheses of these compounds is the oxidation which occurs when oxygen reacts with a solution of $CuCl_2 \cdot DAPSC \cdot 2H_2O$. The oxidation product, Cu(H_2O)(ASCACHOPY)Cl$\cdot \frac{1}{2}H_2O$, contains a hydroxy group on the pyridine ring and is isolated as a mononegative ligand complexed with Cu(II) vide infra. When the solution of $CuCl_2 \cdot DAPSC \cdot 2H_2O$ is prepared under nitrogen using degassed solvent, no oxidation product is obtained. If oxygen is bubbled through a solution of $CuCl_2 \cdot DAPSC \cdot 2H_2O$, the green crystalline oxidation product is obtained. Thus oxygen appears to be the oxidizing agent responsible for this reaction.

Another interesting feature is the production of $[Fe(DAPSC)(H_2O)Cl]Cl \cdot 2H_2O$, an Fe(II) complex, using $FeCl_3 \cdot 6H_2O$ as starting material. The nature of the reducing agent is unknown. This reduction suggested that a Cu(I) species could be present in the preparation of $CuCl_2 \cdot DAPSC \cdot 2H_2O$, but no such species was isolated, even when air was excluded from the reaction.

The order of mixing of reagents does not seem to affect the reactions. Thus the metal salt, DAP, and SCA or PH need only be dissolved in a suitable solvent, usually water, alcohols, or a mixture. The reactants are heated moderately and upon cooling, the product separates. The ligands DAPSC and DAPPH may also be prepared and isolated prior to reaction with metal salts. The template reactions carried out in this work serve to demonstrate the utility and flexibility of such reactions. In several cases, mineral acids must be added in small amounts to suppress deprotonation of the ligand.

IR Spectra. Infrared spectra of compounds studied in this work are listed in Table 2. Peaks characteristic of

2,6-disubstituted pyridine (ring-stretching, 1600-1430 cm^{-1}; ring-breathing, 1000 cm^{-1}; and out-of-plane C-H deformation 780 cm^{-1})[36,37], azomethine (1650-1585 cm^{-1})[37,38], and trimethine (1610-1580 cm^{-1}, 1570-1510 cm^{-1}, and 1490-1430 cm^{-1})[39] appear in all spectra. Characteristic group frequencies for semicarbazone (3400-3120 cm^{-1} and 1620-1560 cm^{-1}, N-H; 1685-1640 cm^{-1}, C=O; 1210-980 cm^{-1}, $-NH_2$; and 785-725 cm^{-1}, $\pi[O{=}C{-}N_2]$)[40] and 2-pyridylhydrazone[41] are present in complexes of DAPSC and DAPPH, respectively. Modes of ionic nitrate (1450-1290 cm^{-1}, ν_3; 1030-980 cm^{-1}, ν_1; 830-810 cm^{-1}, ν_2; and 750-710 cm^{-1}, ν_4),[42] coordinated water (1010-650 cm^{-1}),[43] and lattice water (3550-3200 cm^{-1})[43] are present where appropriate.

UV and Vis Spectra and Magnetic Moments. The ultraviolet and visible spectra and magnetic moments of complexes of DAPSC with some divalent first-row transition metals are listed in Table 3.

The UV spectra cover the region from 50.0kK to 25.0kK. All spectra were recorded using 0.1 M HCl as solvent. Intense charge-transfer bands are the dominant feature of this region. An interesting shift in the absorption peak near 47.0kK is observed. For Mn(II), Fe(II), and Cu(II) the position remains nearly constant, but for Co(II) and Ni(II) the peak shifts to higher energies. According to Orgel,[44] the energy of charge-tranfer bands in this region moves to longer wavelengths as the oxidizing power of the metal ion increases. The relative oxidizing power of the different metals in their complexes with DAPSC should be determinable by observing the shift in this charge-transfer band, but the assignment of the bands in this region is tenuous since metal-chloride charge-transfer bands and ligand absorptions appear in this region. The maxima centered near 42.5kK and 36.0kK remain nearly constant for Mn(II), Cu(II), and Zn(II); but shift to lower energies for Fe(II), Co(II), and Ni(II).

The visible spectra cover the range from 25.0kK to 12.5 kK. The spectra were measured in solution and broad absorption peaks were observed. The Mn(II) complex exhibited no detectable absorption, as expected, since d-d transitions for high spin Mn(II) are spin forbidden. Substantial differences exist between the spectra of complexes with DAPSC and those reported for octahedral complexes.[45-50] A detailed interpretation of the spectra reported in this work may be possible as more PB complexes of transition metals are characterized.

The magnetic moments of complexes with DAPSC are within the ranges normally observed for high spin complexes,[51-57] except in the case of Fe(II) and Co(II) which have moments lower than expected. The moments measured for the Co(II) complex are larger than the spin only value for a d^7 system, a common occurence in Co(II) complexes. The moments for the Fe(II) complex are lower than the spin only value for a d^6 system, an unusual result since no pathway for spin exchange is observed in the structure. The moments measured by the Guoy method are less than those calculated from NMR data. The reason for this difference is unknown, although a change of coordination geometry upon going from the solid state to solution could be responsible.

Table 2
IR SPECTRA OF SELECTED COMPOUNDS

The number of the compound is given at the top of the column containing the respective absorption peaks (in cm^{-1}) and relative intensity (s, strong; m, moderate; w, weak; br, broad). The numbering scheme is: 1, DAPSC; [M(DAPSC)(H_2O)Cl]Cl·2H_2O, 2, M=Mn; 3, M=Fe; 4, M=Co; 5, M=Zn; 6, [Fe(DAPSC)Cl_2]Cl·2H_2O; 7, $NiCl_2$·DAPSC·4H_2O; 8, $CuCl_2$·DAPSC·2H_2O; 9, Cu(H_2O)(ASCACHOPY)Cl·½H_2O; [M(DAPSC)(H_2O)$_2$](NO_3)$_2$·H_2O, 10, M=Mn; 11, M=Ni; 12, M=Cu; [M(DAPPH)(H_2O)$_2$]Cl_2, 13, M=CO; 14, M=Zn.

1	2	3	4	5	6
3480s	3385s	3530m	3505m	3525m	3415m
3300br,m	-	3350s	3355s	3400s	3355s
3200m	3200s	3240s	-	3270s	3300s
-	3040m	3030m	3025m	3030m	3080m
-	-	-	-	-	-
-	-	-	-	-	-
1700s	1680s	1660s	1680s	1680s	1690s
-	1645m	1630m	1640m	-	1665s
-	1605s	1600m	1600m	1605m	1595m
1565s	1540s	1530s	1535s	1535s	1545m
-	-	-	-	-	-
1475w	-	-	-	-	-
1425s	1440m	1440m	1450m	1450m	1450m
1365m	1365s	1365m	1365m	1360m	1380m
1325w	-	-	-	-	-
1290w	1265w	1272w	1270w	1270w	1280w
1250w	1192s	1193s	1195s	1200s	1201s
1155m	-	1161m	1160w	1165w	1162w
1130s	1119w	1118w	1115w	1118w	1120w
1100m	1092m	1091m	1089m	1089m	1092m
990w	1010w	-	1010w	1008w	1015w
-	-	-	-	-	-
858m	823w	-	-	-	-
812m	813w	820m	818m	820m	821m
760w	762w	764w	760w	769w	770w
-	-	-	-	758w	-
-	-	-	-	-	-
650m	-	686w	685w	670br w	-
630w	-	-	-	-	620w
575w	-	-	585w	585br,w	583w
540w	520w	522m	520m	522w	522w
490m	-	-	-	-	-

Table 2 - extended

7	8	9	10	11	12
-	-	-	3500s	3520s	-
3300br,s	3330br,s	3360s	3330br,s	3300br,s	3350br,s
-	-	3260s	-	-	-
-	-	-	-	-	-
-	-	-	2410w	2400w	2410w
-	-	-	2110w	2100w	2095w
1690s	1675s	-	-	-	1760w
1630m	-	1655s	1650br,s	1650br,s	1660s
1605s	1600m	-	1590m	-	1600m
1530s	1535s	1570m	1500m	1510m	1550br,s
-	-	1530m	-	-	-
-	-	-	-	-	-
1450m	1445m	1450m	-	-	-
1355m	1350m	1350s	1380br,s	1375br,s	1360s
-	-	1302s	-	-	-
1272m	1274m	-	1275m	1272m	1278m
1210s	1204s	1225m	1210s	1210s	1210s
1170m	1160m	1148s	1160m	1170m	1165m
1120w	1110w	1120m	1120w	1120w	1110w
1092m	1086m	1095m	1087m	1092m	1090m
-	1012w	1020w	-	-	1015w
-	988w	989w	-	-	990w
-	842w	-	820w	825w	825m
820w	806w	810w	803m	808m	810m
760w	760m	757w	765m	760m	762m
-	-	720w	-	-	-
-	-	-	-	-	-
-	-	-	-	-	-
-	-	620w	-	-	-
578w	600br,m	602m	615br,m	600br,m	595br,m
525m	520m	560br,m	521m	522m	524m
-	-	450w	-	-	-

Table 2 - extended

13	14
-	3500br,m
3350br,s	-
3200br,s	3180br,m
2980m	2990m
-	-
-	-
-	-
1620s	1605s
1580m	1575m
1500m	-
-	-
-	1475m
1430m	1440m
1340w	1330w
-	-
1275s	1270m
1245m	1240s
1195s	1200m
1155m	1145m
1115w	1115w
1085m	1085w
1000w	1000w
-	-
805m	820w
778s	773m
735w	750w
-	695w
-	-
635w	640w
-	590br,w
530w	528w
495w	495w

Table 3
PHYSICAL DATA OF SELECTED COMPOUNDS[a]

COMPOUND	UV, cm^{-1}	VIS, cm^{-1}	Mag. Mom. (Guoy), B.M.	Mag. Mom. (NMR), B.M.
$[Mn(DAPSC)(H_2O)Cl]Cl \cdot 2H_2O$	46,500(5130); 42,000 (2250); 36,200(1740)	- - -	5.92	
$[Fe(DAPSC)(H_2O)Cl]Cl \cdot 2H_2O$	46,300(2070); 36,800 (6100); 29,800(2990)	23,700(31): 22,200(33); 20,100(25); 17,300(23)	4.35	4.85
$[Co(DAPSC)(H_2O)Cl]Cl \cdot 2H_2O$	47,200(4210); 36,800 (9690); 32,200(1720)	18,200(8); 15,800(1)	4.30	4.72
$[Co(DAPSC)(H_2O)_2](NO_3)_2 \cdot H_2O$		18,500(3); 15,800(2)		
$NiCl_2 \cdot DAPSC \cdot 4H_2O$	49,300(13,400); 35,700 (4920); 28,000(819)	14,200(4); 13,000(4)	3.10	
$[Ni(DAPSC)(H_2O)_2](NO_3)_2 \cdot H_2O$		14,100(3); 13,200(4)		3.09
$CuCl_2 \cdot DAPSC \cdot 2H_2O$	46,700(3840); 42,200 (2270); 36,100(2020)	13,200(0.12)	1.63	
$[Cu(DAPSC)(H_2O)_2](NO_3)_2 \cdot H_2O$		13,400(0.13)		
$[Zn(DAPSC)(H_2O)Cl]Cl \cdot 2H_2O$	46,500(5130); 42,000 (2250); 36,200(1740)			
DAPSC	46,900(62,300); 42,600 (18,200); 35,700(26,400)			

[a] - the name of the compound followed by absorption peaks with extinction coefficient in parentheses and the magnetic moments found for some of the compounds are given.

Table 4
ANALYTICAL DATA OF PREPARED COMPOUNDS

COMPOUND	M. W.	M. P.	% C	% H	% N	% Cℓ
			FOUND			
$[Mn(DAPSC)(H_2O)Cl]Cl \cdot 2H_2O$	457.18	355-6°C	28.89	4.58	21.48	15.43
$[Fe(DAPSC)(H_2O)Cl]Cl \cdot 2H_2O$	458.08	>360	28.84	4.48	21.63	
$[Co(DAPSC)(H_2O)Cl]Cl \cdot 2H_2O$	461.17	336	28.57	4.01	21.22	15.15
$[Zn(DAPSC)(H_2O)Cl]Cl \cdot 2H_2O$	467.61	267	28.62	4.38	21.17	16.01
$[Fe(DAPSC)Cl_2]Cl \cdot 2H_2O$	475.52	>360	27.56	3.93	20.32	
$Cu(H_2O)(ASCACHOPY)Cl \cdot \frac{1}{2}H_2O$	361.24	244	33.01	3.64	15.68	
$[Mn(DAPSC)(H_2O)_2](NO_3)_2 \cdot H_2O$	510.28	>360	25.97	4.12	24.49	
$[Ni(DAPSC)(H_2O)_2](NO_3)_2 \cdot H_2O$	514.05	267	25.51	4.05	24.31	
$[Cu(DAPSC)(H_2O)_2](NO_3)_2 \cdot H_2O$	518.88	243	25.07	4.12	23.70	
$[Co(DAPPH)(H_2O)_2]Cl_2$	511.28	>360	44.80	4.41	19.40	14.18
$[Zn(DAPPH)(H_2O)_2]Cl_2$	517.71	230	43.63	4.39	18.11	
$Zn(DAPP) \cdot CHCl_3 \cdot H_2O$	546.16	>360	44.26	3.69	18.01	
$NiCl_2 \cdot DAPSC \cdot 4H_2O$	478.96	320	27.50	5.04	20.35	14.84
$CuCl_2 \cdot DAPSC \cdot 2H_2O$	447.76	203	29.46	4.23	21.94	

Table 4 - extended

% C	% H	% N	% Cℓ
	CALC.		
28.90	4.63	21.45	15.51
28.84	4.62	21.48	
28.65	4.59	21.26	15.38
28.25	4.53	20.97	15.16
27.78	4.03	20.62	
33.25	3.91	15.51	
25.89	4.15	24.70	
25.70	4.12	24.52	
25.46	4.08	24.29	
44.64	4.54	19.18	13.87
44.08	4.48	18.94	
43.98	3.69	17.59	
27.58	4.84	20.47	14.80
29.51	4.28	21.90	

CHAPTER 4

PENTAGONAL BIPYRAMIDAL AND RELATED COMPLEXES OF FIRST-ROW TRANSITION METAL CHLORIDES

Complexes of DAPSC were prepared through template reactions of aqueous solutions of first-row transition metal chlorides and DAP with SCA. The products which crystallized from these reaction mixtures are the subject of this chapter. Manganese(II), cobalt(II), nickel(II), and zinc(II) chlorides react to produce crystalline species which analyze as hydrated complexes of DAPSC with the respective metal ion. Reaction with iron(II) chloride inexplicably yields three products, one of which apparently is an iron(II) complex of DAPSC. Copper(II) chloride yields two products including a green crystalline substance which forms only in the presence of oxygen. The potentially planar pentadentate nature of the DAPSC coupled with the paucity of structures known to contain seven-coordinate transition metal ions prompted an X-ray crystal structure investigation of these complexes.

Structure Solution and Refinement for $[M(DAPSC)(H_2O)Cl]Cl\cdot 2H_2O$ (M=Mn,Fe,Co,Zn)

The Y-coordinate of the zinc atom was determined from a sharpened three-dimensional Patterson map, X and Z were arbitrarily assigned fractional coordinates of ¼. A

Fourier synthesis phased on the zinc atom alone produced one chlorine position, and subsequent Fourier syntheses phased on all located atoms revealed the positions of all non-hydrogen atoms except two lattice water oxygens, O4 and O5, R=0.17. Three cycles of least-squares refinement reduced R to 0.11. A difference Fourier synthesis using these refined coordinates yielded the position of O4. Three cycles of least-squares refinement with anisotropic parameters for the zinc and two chlorine atoms reduced R to 0.10. A difference Fourier synthesis based on these coordinates produced the O5 position. Three least-squares cycles with anisotropic thermal parameters for all atoms reduced R to 0.063. Eleven of the twenty-one hydrogen atoms were located in a subsequent difference Fourier synthesis. The hydrogen atoms were arbitrarily assigned thermal parameters one unit larger than the refined isotropic thermal parameter of the atoms to which they were bonded. After three cycles of least-squares refinement holding the hydrogen atoms constant the shifts of the non-hydrogen atoms were less than one-tenth of their respective standard deviations and the structure was considered refined, R=0.058.

The similarity of the preliminary photographs and refined cell constant data for the analogous Mn(II), Fe(II), and Co(II) compounds suggested that these structures were isomorphous to the Zn(II) compound.

A Patterson map calculated from the Co(II) data was essentially identical to that for Zn(II). A Fourier synthesis using the refined isotropic zinc and chlorine positions indicated that the structures were indeed isomorphous, R=0.36. Three cycles of least-squares refinement using the refined isotropic parameters from the zinc compound reduced R to 0.088. Three least-squares cycles with anisotropic thermal parameters reduced R to 0.046. A difference Fourier synthesis using these refined positions revealed thirteen hydrogen atoms. The hydrogens were arbitrarily assigned thermal parameters one unit larger than the refined isotropic thermal parameters of the atoms to which they were bonded. After three cycles of least-squares refinement the shifts of all non-hydrogen atoms were less than one-tenth of their respective standard deviations and the refinement was terminated, R=0.039.

After three cycles of least-squares refinement of the Fe(II) structure using the refined anisotropic Co(II) parameters as a starting set, the shifts of all atoms were less than one-tenth of their respective standard deviations and the structure was considered solved, R=0.040

A difference Fourier calculated with the Mn(II) data using refined isotropic Co(II) coordinates revealed no discrepancies, R=0.18. Three least-squares cycles using the refined isotropic Co(II) parameters followed by three least-squares cycles using anisotropic thermal parameters reduced R to 0.039. A difference Fourier synthesis using the refined anisotropic parameters revealed the locations of all twenty-one hydrogen atoms. The hydrogen atoms were assigned thermal parameters one unit larger than the refined isotropic thermal parameters of the bonded atoms. All shifts were less than one-tenth of their respective standard deviations and refinement was terminated.

Results for [M(DAPSC)(H_2O)Cl]Cl·2H_2O (M=Mn,Fe,Co,Zn)

Final positional and thermal parameters for the non-hydrogen atoms of the four structures are given in Table 5. The probable positional parameters and carbon-hydrogen distances for the hydrogen atoms of [Mn(DAPSC)(H_2O)Cl]Cl·2H_2O are given in Table 6. Intramolecular bond distances and angles and short intermolecular contacts are listed in Table 7. Least-squares planes and deviations are compared in Table 8. The observed and calculated structure factors are in Table 9. The complex ion and atoms numbering scheme are shown in Figure 2, an ORTEP[58] diagram. Figure 3 is an ORTEP[58] stereo packing diagram of the unit cell contents.

Discussion

The four compounds form an isomorphous series, differing only in the nature of the central metal atom. The pentagonal bipyramidal geometry of the complexes is easily seen in Figure 2. Atoms O1, O2, N1, N2, and N5 form a planar pentagonal array with chloride and water occupying the apices. Figure 3 illustrates the hydrogen bonding and molecular arrangement in the unit cell.

The metal-DAPSC bond distances in these complexes are

Table 5

FINAL POSITIONAL AND THERMAL PARAMETERS ($\times 10^4$) FOR THE NON-HYDROGEN ATOMS OF $[M(DAPSC)(H_2O)Cl]Cl \cdot 2H_2O$ (M = Mn, Fe, Co, Zn) WITH THEIR RESPECTIVE ESTIMATED STANDARD DEVIATIONS IN PARENTHESES

The coordinates of the atoms for each structure are listed according to the order of the metal atoms.

Atom	X	Y	Z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
M = Mn	2500*	10507(1)	2500*	16(1)	22(1)	116(2)	-1(1)	32(1)	2(3)
Fe	2500*	10457(1)	2500*	14(1)	20(1)	100(1)	-1(1)	27(1)	2(2)
Co	2500*	10437(1)	2500*	13(1)	17(1)	91(1)	-2(1)	26(1)	1(2)
Zn	2500*	10452(1)	2500*	14(1)	27(1)	70(2)	-2(1)	1(2)	1(3)
Cℓ1	3420(2)	10355(2)	5199(4)	25(1)	38(2)	134(5)	1(2)	9(3)	7(5)
	3420(1)	10320(1)	5191(3)	22(1)	34(1)	118(3)	2(1)	4(2)	2(3)
	3401(1)	10310(2)	5187(3)	23(1)	34(1)	120(4)	-1(2)	9(2)	-4(3)
	3385(2)	10337(3)	5150(4)	15(1)	29(2)	48(5)	2(2)	-21(4)	-4(5)
Cℓ2	342(2)	5668(2)	4171(4)	21(1)	49(2)	234(5)	9(2)	62(4)	14(5)
	352(1)	5698(2)	4170(3)	19(1)	44(1)	216(3)	4(1)	57(2)	22(3)
	345(2)	5724(2)	4162(3)	18(1)	42(1)	218(4)	2(2)	68(3)	18(4)
	339(2)	5692(3)	4144(5)	11(1)	40(2)	136(7)	6(3)	22(4)	19(7)
O1	3118(4)	11762(5)	1540(10)	23(2)	27(5)	201(13)	-5(6)	73(10)	11(14)
	3103(3)	11749(4)	1635(7)	23(2)	30(3)	163(9)	-1(4)	50(6)	1(9)
	3078(4)	11735(5)	1660(8)	20(2)	27(4)	174(10)	-4(5)	50(8)	1(11)
	3084(5)	11744(7)	1607(13)	14(3)	26(6)	100(16)	2(7)	26(12)	1(16)
O2	1882(4)	11778(5)	3441(10)	22(3)	30(5)	175(14)	-12(6)	72(10)	1(13)
	1937(3)	11745(4)	3445(7)	19(2)	27(3)	154(9)	-4(4)	56(6)	-4(9)
	1952(3)	11740(5)	3473(8)	21(2)	31(4)	151(10)	-6(5)	69(8)	-1(11)

Table 5 - continued

Atom	X	Y	Z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
	1922(5)	11754(6)	3449(12)	18(4)	22(6)	86(16)	-9(7)	28(13)	2(16)
O3	2341(5)	13774(6)	2509(13)	59(4)	38(5)	195(14)	2(7)	104(12)	12(17)
	2386(4)	13776(4)	2572(10)	59(3)	38(4)	180(10)	7(5)	116(9)	9(12)
	2376(5)	13777(5)	2606(12)	53(3)	53(4)	165(12)	7(6)	110(10)	-18(15)
	2356(7)	13776(7)	2590(14)	48(6)	35(6)	101(16)	-9(10)	69(15)	2(19)
O4	1726(4)	10673(5)	88(10)	26(2)	46(5)	126(13)	-6(5)	8(9)	8(13)
	1758(3)	10642(4)	133(7)	22(2)	43(3)	121(9)	-9(4)	12(6)	4(9)
	1744(4)	10651(5)	172(8)	20(2)	41(4)	127(11)	-6(5)	18(8)	1(11)
	1752(5)	10654(7)	177(11)	17(3)	37(6)	74(15)	2(7)	-4(11)	-7(15)
O5	4933(5)	5774(7)	1035(11)	28(3)	76(6)	276(17)	-27(7)	96(12)	7(17)
	4956(4)	5799(5)	1077(9)	22(3)	68(4)	260(12)	-29(6)	88(9)	17(12)
	4947(5)	5802(7)	1062(11)	22(3)	76(5)	262(15)	-30(7)	113(11)	22(15)
	4933(6)	5788(9)	1060(15)	19(4)	63(7)	202(23)	-18(9)	50(15)	8(22)
N1	2426(5)	8746(5)	2313(12)	21(2)	28(4)	125(14)	-3(8)	12(9)	-20(16)
	2449(4)	8767(4)	2344(9)	17(2)	26(3)	113(9)	-3(5)	17(6)	-15(11)
	2447(5)	8775(4)	2340(11)	24(2)	21(3)	103(10)	-7(6)	32(7)	6(13)
	2444(6)	8756(6)	2315(14)	12(3)	19(5)	55(17)	-4(10)	4(11)	-8(19)
N2	3418(5)	9837(7)	1209(11)	25(3)	27(6)	134(15)	6(7)	47(10)	-1(14)
	3427(3)	9855(5)	1277(7)	20(2)	26(4)	128(10)	-3(4)	37(7)	-2(10)
	3430(4)	9868(6)	1308(9)	20(3)	26(5)	125(12)	-5(6)	47(9)	12(12)
	3420(6)	9838(9)	1235(13)	15(4)	18(7)	72(18)	-4(8)	15(13)	1(18)
N3	3885(6)	10537(6)	746(14)	22(3)	34(6)	183(14)	-4(7)	78(10)	26(15)
	3901(5)	10571(5)	800(11)	21(2)	26(4)	187(9)	-7(4)	68(7)	8(10)
	3888(6)	10585(6)	838(13)	17(2)	26(5)	173(11)	-2(6)	64(9)	-3(12)
	3886(9)	10562(8)	787(19)	19(4)	19(7)	94(18)	-4(9)	32(13)	7(18)

Table 5 - continued

Atom	X	Y	Z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
N4	4097(5)	12236(8)	276(13)	31(4)	31(7)	259(21)	-7(8)	49(13)	66(18)
	4076(4)	12274(6)	373(9)	31(3)	34(5)	235(15)	-7(6)	65(9)	58(13)
	4045(5)	12288(7)	424(11)	19(3)	34(6)	244(18)	-1(7)	80(12)	47(15)
	4054(7)	12256(10)	370(17)	26(5)	33(8)	159(30)	2(10)	45(19)	71(24)
N5	1506(4)	9872(6)	3492(10)	17(2)	26(6)	129(14)	-3(6)	35(9)	-14(13)
	1530(3)	9884(5)	3523(7)	14(2)	27(4)	112(10)	1(4)	26(7)	-15(10)
	1525(4)	9890(6)	3533(9)	15(2)	32(5)	107(12)	-2(5)	27(9)	-4(12)
	1506(5)	9877(8)	3493(12)	9(3)	20(7)	46(16)	-4(8)	-4(11)	-8(17)
N6	1046(5)	10584(6)	4057(12)	26(3)	24(7)	174(16)	-6(7)	33(11)	-20(14)
	1085(4)	10605(5)	4075(8)	21(2)	29(4)	136(11)	-7(4)	37(8)	-19(10)
	1080(5)	10622(6)	4058(10)	23(3)	26(5)	156(13)	3(6)	52(10)	-21(12)
	1062(6)	10609(8)	4026(15)	8(4)	28(8)	96(20)	-4(8)	12(13)	-18(18)
N7	928(5)	12280(8)	4716(13)	24(3)	49(7)	190(20)	13(8)	97(13)	-16(18)
	984(4)	12301(5)	4730(9)	26(2)	37(5)	179(13)	3(5)	72(9)	-30(12)
	997(5)	12306(7)	4742(11)	30(3)	30(6)	223(16)	-14(7)	87(11)	-21(14)
	968(6)	12291(9)	4725(15)	14(4)	25(7)	137(24)	6(9)	35(15)	-28(21)
C1	2976(5)	8219(7)	1764(13)	24(3)	13(6)	118(16)	-1(7)	16(12)	2(15)
	2996(4)	8241(5)	1787(9)	24(2)	21(4)	93(10)	4(4)	21(7)	-20(9)
	3003(5)	8251(6)	1802(10)	12(3)	25(5)	83(12)	3(5)	4(9)	-18(11)
	2984(7)	8231(9)	1784(15)	14(4)	18(8)	42(19)	-3(9)	-16(15)	-3(18)
C2	2977(6)	7152(8)	1733(14)	29(4)	38(8)	138(19)	-9(8)	25(14)	-24(18)
	2997(4)	7172(6)	1743(10)	28(2)	28(5)	134(13)	-3(5)	34(9)	-2(12)
	2998(5)	7197(7)	1762(12)	30(3)	27(6)	133(16)	11(7)	36(11)	-1(14)
	2995(7)	7173(11)	1757(16)	16(5)	29(10)	54(21)	-1(11)	8(16)	-11(21)
C3	2401(7)	6637(7)	2271(16)	37(4)	31(6)	138(21)	-6(9)	21(15)	7(21)

Table 5 - continued

Atom	X	Y	Z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
	2428(5)	6660(5)	2301(11)	35(3)	24(4)	134(13)	-13(6)	23(9)	16(14)
	2408(6)	6684(7)	2324(14)	34(3)	19(5)	146(16)	-20(8)	26(12)	-17(17)
	2412(9)	6670(9)	2281(17)	30(5)	21(7)	60(22)	-8(13)	-29(17)	2(24)
C4	1834(6)	7190(9)	2858(14)	28(4)	28(8)	138(19)	-2(8)	35(14)	7(18)
	1862(4)	7204(6)	2886(10)	21(2)	21(5)	132(13)	-5(5)	24(9)	11(12)
	1853(6)	7211(8)	2889(12)	31(3)	25(6)	128(16)	-10(7)	40(11)	20(14)
	1839(7)	7199(10)	2863(17)	19(5)	21(8)	68(22)	-11(9)	-2(17)	-5(20)
C5	1374(5)	8247(8)	2842(13)	19(3)	34(7)	95(17)	-11(7)	20(12)	5(16)
	1895(4)	8260(5)	2883(9)	14(2)	31(4)	89(11)	-2(5)	4(8)	2(10)
	1877(5)	8273(7)	2882(11)	18(3)	26(5)	107(14)	-1(6)	7(10)	7(13)
	1872(7)	8260(9)	2856(14)	14(4)	18(8)	24(18)	-3(9)	-11(14)	6(18)
C6	3553(6)	8869(9)	1207(14)	27(4)	34(8)	119(20)	1(9)	12(13)	-48(18)
	3582(4)	8897(6)	1222(10)	22(2)	25(5)	119(12)	-2(5)	15(8)	-15(11)
	3583(5)	8910(7)	1221(12)	25(3)	22(5)	104(14)	4(6)	27(10)	-7(14)
	3569(7)	8873(11)	1226(16)	11(4)	30(10)	52(21)	-4(10)	14(15)	-48(21)
C7	4251(7)	8409(10)	660(17)	23(5)	55(9)	294(25)	28(10)	71(17)	11(23)
	4274(5)	8463(7)	667(12)	20(3)	37(6)	272(16)	8(6)	56(11)	-37(15)
	4270(7)	8472(9)	615(15)	27(4)	48(7)	233(19)	3(8)	46(14)	-26(18)
	4270(8)	8443(12)	686(22)	11(5)	40(10)	188(33)	21(10)	26(19)	-7(27)
C8	3662(6)	11551(8)	882(14)	21(4)	47(8)	112(21)	-1(8)	28(16)	-11(19)
	3652(4)	11570(5)	945(9)	17(2)	37(4)	129(12)	-1(5)	37(9)	-10(11)
	3633(5)	11569(7)	983(11)	17(3)	33(5)	114(15)	-9(6)	17(11)	-1(14)
	3634(7)	11546(10)	936(15)	12(5)	33(10)	49(23)	-8(11)	-6(17)	-2(23)
C9	1322(5)	8921(8)	3455(12)	20(3)	40(7)	107(17)	-12(7)	24(12)	-8(16)
	1334(4)	8932(6)	3512(9)	19(2)	32(4)	99(11)	-10(5)	31(8)	2(11)

Table 5 - continued

Atom	X	Y	Z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
	1327(5)	8948(7)	3510(11)	18(3)	36(5)	96(14)	-12(6)	16(10)	9(13)
	1311(6)	8948(10)	3467(14)	9(4)	24(9)	32(18)	-3(9)	-22(13)	-15(20)
C10	627(7)	8489(9)	3942(16)	27(4)	47(7)	204(21)	-27(9)	84(15)	11(20)
	631(5)	8537(6)	4012(11)	22(3)	42(5)	174(13)	-16(6)	65(10)	7(12)
	626(6)	8548(8)	4039(13)	17(3)	35(6)	168(16)	-8(7)	59(12)	40(15)
	620(9)	8538(12)	3949(19)	20(5)	31(10)	121(26)	-21(11)	36(19)	8(25)
C11	1331(6)	11575(8)	4056(14)	21(4)	25(7)	156(19)	3(8)	10(14)	-23(18)
	1374(4)	11573(5)	4064(9)	17(2)	27(4)	115(12)	2(5)	23(9)	-12(11)
	1384(5)	11578(7)	4101(11)	14(3)	28(5)	105(15)	-3(6)	21(11)	5(14)
	1355(7)	11590(10)	4044(16)	14(5)	25(10)	46(23)	-3(10)	-5(17)	12(22)

* Coordinate determined arbitrarily

Table 6
FINAL POSITIONAL AND THERMAL PARAMETERS (x 10^3) FOR THE HYDROGEN ATOMS OF
$[Mn(DAPSC)(H_2O)Cl]Cl \cdot 2H_2O$

ATOM	BONDED TO	DISTANCE, Å	X	Y	Z	B(Å²)
H1	N4	1.10	393	1299	68	4.8
H2	N4	1.01	455	1204	-22	4.8
H3	N3	1.01	431	1043	10	3.6
H4	N7	0.94	52	1209	523	4.6
H5	N7	0.91	113	1291	490	4.6
H6	N6	1.05	65	1039	481	3.9
H7	C7	1.08	435	885	-40	5.3
H8	C7	0.98	450	792	149	5.3
H9	C7	1.07	480	869	113	5.3
H10	C10	1.08	42	879	501	4.5
H11	C10	0.94	26	882	316	4.5
H12	C10	0.89	53	785	422	4.5
H13	C2	1.09	347	674	151	4.0
H14	C3	1.01	252	588	237	4.3
H15	C4	1.13	148	668	352	4.0
H16	O3	0.85	239	1313	256	5.6
H17	O3	0.93	277	1400	216	5.6
H18	O4	1.01	193	1057	-98	4.4
H19	O4	0.97	133	1114	-38	4.4
H20	O5	0.88	511	597	14	6.0
H21	O5	0.84	449	560	73	6.0

Table 7
INTRAMOLECULAR BOND DISTANCES AND ANGLES AND SHORT INTERMOLECULAR CONTACTS FOR
$[M(DAPSC)(H_2O)Cl]Cl \cdot 2H_2O$ (M=Mn,Fe,Co,Zn)
WITH THEIR ESTIMATED STANDARD DEVIATIONS IN PARENTHESES

(a) Bond Distances (Å)

	M=Mn	Fe	Co	Zn
M-Cl	2.532(3)	2.507(2)	2.479(2)	2.433(3)
M-O1	2.212(7)	2.192(5)	2.161(6)	2.184(9)
M-O2	2.220(7)	2.175(5)	2.138(6)	2.207(9)
M-O4	2.222(8)	2.153(6)	2.141(6)	2.121(9)
M-N1	2.310(7)	2.220(5)	2.188(5)	2.229(8)
M-N2	2.303(9)	2.229(6)	2.200(7)	2.247(10)
M-N5	2.273(8)	2.195(6)	2.182(7)	2.222(10)
O1-C8	1.241(13)	1.240(9)	1.241(11)	1.239(16)
O2-C11	1.231(13)	1.230(9)	1.227(10)	1.224(16)
N1-C1	1.358(13)	1.345(9)	1.343(11)	1.325(16)
N1-C5	1.335(14)	1.335(10)	1.353(12)	1.357(16)
N2-N3	1.351(13)	1.371(10)	1.355(12)	1.358(17)
N2-C6	1.290(14)	1.290(10)	1.291(12)	1.294(18)
N3-C8	1.398(13)	1.398(10)	1.368(12)	1.381(18)
N4-C8	1.348(15)	1.331(11)	1.331(12)	1.331(18)
N5-N6	1.385(12)	1.365(9)	1.358(11)	1.367(15)
N5-C9	1.288(12)	1.297(10)	1.290(12)	1.267(17)
N6-C11	1.397(13)	1.373(9)	1.383(11)	1.389(17)
N7-C11	1.350(15)	1.351(10)	1.334(12)	1.331(17)
C1-C2	1.395(14)	1.402(10)	1.390(12)	1.387(18)
C1-C6	1.488(15)	1.495(10)	1.489(12)	1.481(18)
C2-C3	1.385(16)	1.367(12)	1.383(15)	1.369(21)
C3-C4	1.413(16)	1.395(12)	1.375(15)	1.395(21)
C4-C5	1.385(15)	1.386(11)	1.388(12)	1.392(18)
C5-C9	1.492(14)	1.497(10)	1.485(12)	1.503(17)
C6-C7	1.545(18)	1.510(12)	1.507(12)	1.517(20)
C9-C10	1.507(16)	1.489(11)	1.489(14)	1.471(20)

Table 7 - continued

(b) Bond Angles (°)

	M=Mn	Fe	Co	Zn
Cℓ1-M-O1	93.4(2)	92.1(1)	92.8(2)	93.3(3)
Cℓ1-M-O2	93.6(2)	91.9(1)	90.6(2)	91.1(2)
Cℓ1-M-O4	177.8(2)	176.4(2)	176.6(2)	176.2(3)
Cℓ1-M-N1	90.1(2)	89.6(2)	89.9(2)	90.7(3)
Cℓ1-M-N2	86.3(2)	85.3(2)	85.8(2)	87.4(3)
Cℓ1-M-N5	96.8(2)	96.1(2)	95.4(2)	96.2(3)
O1-M-O2	83.6(3)	78.4(2)	76.4(2)	78.5(3)
O1-M-O4	84.5(3)	84.3(2)	83.9(2)	83.1(4)
O1-M-N1	138.1(3)	140.5(2)	141.9(3)	140.4(4)
O1-M-N2	70.3(3)	71.4(2)	72.0(3)	71.9(4)
O1-M-N5	152.5(3)	149.0(2)	146.7(3)	148.2(4)
O2-M-O4	86.8(3)	87.9(2)	87.4(2)	86.8(3)
O2-M-N1	137.8(3)	141.0(2)	141.6(3)	140.9(4)
O2-M-N2	153.9(3)	149.5(2)	148.0(3)	150.2(4)
O2-M-N5	70.3(3)	71.5(2)	71.4(2)	71.1(3)
O4-M-N1	91.1(3)	92.8(2)	93.4(3)	93.0(4)
O4-M-N2	92.3(2)	92.9(2)	94.3(3)	92.8(4)
O4-M-N5	85.4(3)	87.3(2)	86.7(2)	86.2(4)
N1-M-N2	68.3(3)	69.4(2)	70.3(3)	68.9(4)
N1-M-N5	67.5(3)	69.6(2)	70.4(3)	69.9(4)
N2-M-N5	135.7(3)	139.0(2)	140.6(3)	138.7(4)
M-O1-C8	119.0(7)	118.4(5)	117.5(6)	116.9(8)
M-O2-C11	118.8(7)	118.0(5)	118.2(6)	118.7(8)
M-N1-C1	119.3(7)	120.3(5)	120.0(6)	120.9(8)
M-N1-C5	120.3(7)	120.3(5)	120.2(6)	119.0(8)
C1-N1-C5	120.2(9)	119.3(6)	119.7(7)	120.0(10)
M-N2-N3	114.7(7)	115.8(5)	115.2(6)	114.3(9)
M-N2-C6	122.0(7)	123.0(5)	122.6(6)	121.6(9)
N3-N2-C6	122.2(9)	120.5(7)	121.6(8)	122.9(12)
N2-N3-C8	114.4(9)	113.1(7)	113.8(9)	113.7(12)
M-N5-N6	116.3(6)	116.0(4)	116.3(5)	115.5(7)
M-N5-C9	124.5(6)	124.2(5)	123.3(6)	124.0(8)

Table 7 - continued

	M=Mn	Fe	Co	Zn
N6-N5-C9	119.0(8)	119.5(6)	120.2(7)	120.3(10)
N5-N6-C11	112.0(8)	113.1(6)	113.6(7)	114.2(10)
N1-C1-C2	121.1(9)	121.7(6)	120.8(8)	122.6(11)
N1-C1-C6	114.6(9)	114.0(6)	114.0(7)	114.0(11)
C2-C1-C6	124.2(9)	124.3(6)	125.1(8)	123.4(11)
C1-C2-C3	118.5(10)	118.6(7)	119.1(9)	117.6(12)
C2-C3-C4	120.1(11)	119.8(8)	120.3(9)	121.4(13)
C3-C4-C5	117.7(10)	118.4(7)	118.1(9)	117.4(12)
N1-C5-C4	122.4(10)	122.2(7)	121.9(8)	121.1(11)
N1-C5-C9	114.5(9)	114.0(6)	113.3(7)	114.3(10)
C4-C5-C9	123.1(9)	123.7(7)	124.7(8)	124.6(11)
N2-C6-C1	114.3(9)	112.3(6)	112.2(8)	113.2(11)
N2-C6-C7	123.5(10)	125.0(7)	125.6(9)	123.3(12)
C1-C6-C7	122.2(10)	122.7(7)	122.2(8)	123.5(12)
O1-C8-N3	120.9(10)	120.6(7)	120.9(9)	122.3(12)
O1-C8-N4	125.4(10)	125.2(7)	123.0(9)	123.6(12)
N3-C8-N4	113.7(10)	114.0(7)	116.0(9)	114.0(12)
N5-C9-C5	112.8(9)	111.6(6)	112.7(8)	112.5(10)
N5-C9-C10	125.8(9)	125.3(7)	125.4(8)	126.3(12)
C5-C9-C10	121.3(9)	123.1(6)	121.9(8)	121.2(11)
O2-C11-N6	122.2(10)	121.0(7)	119.7(8)	120.1(12)
O2-C11-N7	123.9(10)	123.8(7)	124.9(8)	125.3(12)
N6-C11-N7	113.8(9)	115.2(7)	115.2(8)	114.6(12)

Table 7 - continued

(c) Short Intermolecular Contacts (Å)

ATOM A	EQUIV.POS.	ATOM B	EQUIV.POS.	DISTANCE			
				M=Mn	Fe	Co	Zn
O5	X,Y,Z	Cℓ1	X,1½-Y,Z-½	3.111(9)	3.118(7)	3.097(8)	3.127(11)
O3	X,Y,Z	Cℓ1	X,2½-Y,Z-½	3.164(10)	3.131(7)	3.124(9)	3.159(12)
O5	X,Y,Z	Cℓ2	½+X,1-Y,Z	3.155(9)	3.159(7)	3.162(9)	3.137(12)
N3	X,Y,Z	Cℓ2	½+X,½+Y,Z-½	3.159(11)	3.133(9)	3.145(11)	3.146(16)
O4	X,Y,Z	Cℓ2	X,1½-Y,Z-½	3.067(8)	3.080(6)	3.078(7)	3.090(10)
O4	X,Y,Z	O3	X,2½-Y,Z-½	2.647(12)	2.633(9)	2.653(11)	2.629(15)
O5	X,Y,Z	N6	½+X,Y-½,Z-½	2.819(12)	2.822(10)	2.848(11)	2.844(16)

Table 8
LEAST-SQUARE PLANES AND DEVIATIONS FOR [M(DAPSC)(H_2O)Cl]Cl·$2H_2O$ (M=Mn,Fe,Co,Zn)

The titles of the plane are followed by the deviations (x 10^3 Å) of the atoms listed in the left-hand column. The atoms used to define the plane are denoted by asterisks. The equation of the plane is ax+by+cz=d, where d is the distance (Å) from the origin. The dihedral angles are in degrees and decimal fractions.

Plane 1. Plane Through the Planar Pentagonal Donor Set

ATOM	Mn	Fe	Co	Zn
M	84	41	33	68
Cℓ1	2609	2541	2505	2498
O1*	-93	-96	-116	-104
O2*	97	100	115	112
O4	-2134	-2108	-2096	-2047
N1*	7	5	-1	14
N2*	61	61	76	60
N5*	-72	-70	-74	-82
a	0.4582	0.4582	0.4594	0.4580
b	-0.0459	-0.0482	-0.0517	-0.0495
c	0.8877	0.8876	0.8867	0.8876
d	2.9985	2.9776	2.9220	2.9154

Plane 2. Plane Through the Pyridine Ring

ATOM	MN	Fe	Co	Zn
M	141	103	111	130
O1	-129	-104	-104	-122
O2	347	336	390	376
N1*	-2	-1	-4	-2
N2	-115	-86	-77	-121
N5	165	152	180	167
C1*	1	3	7	-2
C2*	3	-3	-4	7
C3*	-6	1	-2	-8
C4*	5	1	6	4

Table 8 - continued

ATOM	Mn	Fe	Co	Zn
C5*	-1	-1	-2	1
a	0.3702	0.3781	0.3704	0.3650
b	-0.0155	-0.0167	-0.0139	-0.0142
c	0.9288	0.9256	0.9288	0.9309
d	3.0694	3.0880	3.0762	3.0377

Dihedral Angle Between Planes 1 and 2

	Mn	Fe	Co	Zn
Angle	5.83	5.39	6.04	6.21

Table 9
OBSERVED AND CALCUATED STRUCTURE FACTORS FOR $[M(DAPSC)(H_2O)Cl]Cl \cdot 2H_2O$ (M=Mn,Fe,Co,Ni)

The structure factors for the reflection (HKL) are listed to the right of the appropriate L value under the corresponding H and K values. FO and FC refer to F_{obs} and F_{calc} respectively. The phase angle for each reflection is listed under the heading ALPHA. The structure factors for the Mn compound appear first, followed by those for the Fe, Co, and Zn compounds, respectively.

```
   L     FO      FC   ALPHA

H=     0,  K=     0

   2    116      83    2.14
   4    236     246    0,19
   6    211     204    2.73
   8    188     190    0.35

H=     2,  K=     0

   0    731     943    3.08
   2   1617    2534   -0.22
   4    395     382   -2.92
   6     88      96   -1.12
   8    123     121   -3.04
  -8    198     201   -3.11
  -6    -21      28    0.33
  -4    725     764    3.10
  -2    231     178   -3.05

H=     4,  K=     0

   0    227     215    1.51
   2   1068    1182    2.90
   4    805     846   -0.52
   6    272     280   -3.13
   8    -24      17   -2.08
  -8    175     175    0.0
  -6    366     366    3.03
  -4    104     103    2.03
  -2    840     916    2.85

H=     6,  K=     0

   0    367     354    1.47
   2    548     579    0.38
   4    546     552    2.64
   6    366     368   -0.46
  -8     78      71   -2.39
  -6    398     415   -0.32
  -4    357     371   -2.91
  -2    373     392    0.09

H=     8,  K=     0

   0    265     259    0.08
   2     87      93    2.72
   4    235     234   -0.45
   6    251     265    3.04
  -8    179     173    0.08
  -6    329     325   -2.99
  -4    275     287   -0.85
  -2    619     671   -2.99

H=    10,  K=     0

   0    433     464    2.72
   2    243     253    0.53
   4    122     117   -2.87
   6     98     100   -0.91
  -8    147     148    3.07
  -6    314     323    0.10
  -4    472     486   -3.14
  -2    190     168   -0.55

H=    12,  K=     0

   0    363     371    0.32
   2    285     287    1.73
   4    283     302    0.52
  -6    151     157    3.13
  -4    522     529   -0.20
  -2    277     280   -3.13

H=    14,  K=     0

   0    326     326   -2.95
   2    123     128    0.01
   4     81      86    2.77
  -6    187     191   -0.26
```

```
   L     FO      FC   ALPHA

  -4    448     451   -2.96
  -2    383     396   -0.80

H=    16,  K=     0

   0    175     188   -0.89
   2    230     235    2.99
  -6    144     133    2.68
  -4    182     191   -0.62
  -2    477     486   -3.06

H=    18,  K=     0

   0    249     251    2.82
   2    132     133    0.15
  -4    -25      31    1.94
  -2    290     294   -0.50

H=     0,  K=     1

   1    714     800    1.53
   3    172     180   -1.47
   5    144     155   -2.99
   7    202     198   -2.04

H=     1,  K=     1

   0    179     168   -2.78
   2    490     504    2.91
   4     90      94   -1.87
   6     45      59    0.14
   8    -24      35    2.67
  -8     97      92    3.13
  -6     49      60    1.66
  -4    152     167    2.77
  -2    205     190   -2.89

H=     2,  K=     1

   1    760     838   -1.50
   3    591     584    1.37
   5     97      85    1.57
   7    212     218    2.16
  -7    161     163   -1.11
  -5    392     388    1.58
  -3    457     447    1.52
  -1    454     423    1.28

H=     3,  K=     1

   0    167     114   -2.83
   2    431     467   -2.62
   4    318     324    2.70
   6    -23      41   -1.90
   8     44      42    0.12
  -8     63      55   -0.14
  -6    128     130   -3.07
  -4    125     123    0.24
  -2     80      75    0.87

H=     4,  K=     1

   1    335     326   -1.04
   3    965    1025   -1.45
   5    186     175    0.43
   7    109     110   -0.58
  -7     62      64   -2.79
  -5    444     444   -1.65
  -3    314     293    1.91
  -1    116      91    0.0

H=     5,  K=     1

   0    282     260    0.12
   2    108     103    0.0
   4    212     228   -2.37
   6    162     167    2.09
  -8     99      93   -2.97
  -6    118     118   -0.29
  -4     51      47    3.04
```

```
   L     FO      FC   ALPHA

  -2    449     465    0.02

H=     6,  K=     1

   1     78      56    0.80
   3     51      23    0.94
   5    474     481   -1.76
   7     43      27    1.69
  -7    182     183   -1.78
  -5    225     228    2.27
  -3    248     255   -2.34
  -1    679     656    1.98

H=     7,  K=     1

   0    375     376   -0.14
   2     85      71   -1.41
   4     76      84   -0.34
   6    134     138   -2.14
  -8     58      49   -0.46
  -6    211     217    3.02
  -4     76      73   -0.16
  -2    109     107    1.62

H=     8,  K=     1

   1    609     631    1.72
   3    145     146    0.79
   5    220     214    1.72
   7    163     164   -2.41
  -7    136     125    0.87
  -5    211     206   -1.34
  -3    522     540    1.79
  -1    202     188    2.48

H=     9,  K=     1

   0    161     161    1.14
   2    209     217   -0.33
   4     57      49   -2.04
   6     68      72    0.23
  -8     94      99    0.83
  -6     83      85   -0.33
  -4    255     258    2.90
  -2     93     102    0.59

H=    10,  K=     1

   1    301     287   -1.33
   3    207     208    0.67
   5    213     207   -0.47
  -7    263     267   -1.29
  -5     79      85   -1.17
  -3    427     415   -1.56
  -1    287     276    1.80

H=    11,  K=     1

   0    102     100    1.07
   2     82      87    1.40
   4     99     102   -0.43
   6    -25      18    3.05
  -6     66      57    0.49
  -4    115     109   -0.24
  -2    216     218    2.60

H=    12,  K=     1

   1    273     270    2.01
   3    221     213   -1.60
   5    -25      35    0.90
  -7    163     161    1.64
  -5    293     297   -1.44
  -3    184     182    2.48
  -1    275     273   -2.32

H=    13,  K=     1

   0    165     171    2.71
   2    -24      32   -3.03
```

```
    L     FO      FC    ALPHA

    4     55      47    -3.00
   -6    199     196    -2.79
   -4     55      68    -2.26
   -2     48      42     0.33

 H=   14,  K=    1

    1    129     133     3.08
    3    258     255     1.74
   -7    112     109    -0.73
   -5    231     235     1.17
   -3    207     203    -1.45
   -1    365     361     2.11

 H=   15,  K=    1

    0     95      96     0.93
    2     59      65     2.46
    4    -25      10    -1.49
   -6     43      50    -0.54
   -4    133     127    -2.87
   -2     48      67    -1.99

 H=   16,  K=    1

    1    126     131     1.73
    3     90      89    -0.72
   -5    289     288    -1.09
   -3    125     138     0.55
   -1    295     289    -1.51

 H=   17,  K=    1

    0     42      36    -1.54
    2     88      95     0.89
   -4     98      98    -0.45
   -2    -25      41     1.54

 H=   18,  K=    1

    1    210     208    -2.01
   -3    239     242    -1.48
   -1     98      92     2.07

 H=   19,  K=    1

    0     63      63     1.14
   -2     66      58    -0.91

 H=    0,  K=    2

    0    566     534     0.0
    2    198     196    -0.45
    4    179     188     0.54
    6    192     192     2.72
    8    155     151     0.12

 H=    1,  K=    2

    1    375     357    -1.40
    3    124     126    -3.09
    5    134     127     2.48
    7    144     149     1.58
   -7    -23       6     0.85
   -5    231     223     1.44
   -3    165     150     0.53
   -1     83      76    -0.74

 H=    2,  K=    2

    0    119     135    -2.09
    2    170     185    -1.06
    4    340     345    -2.25
    6     42      49    -1.00
    8     96     103    -2.95
   -8    169     171    -2.77
   -6    142     139     0.31
   -4    554     552    -3.08
   -2    121     110    -2.43
```

```
    L     FC      FC    ALPHA

 H=    3,  K=    2

    1    216     193    -1.11
    3    355     362    -1.23
    5     98     103    -2.21
    7     61      59    -1.61
   -7     35      45    -3.09
   -5     35      23    -2.19
   -3     25      16     1.85
   -1    398     389    -1.18

 H=    4,  K=    2

    0    336     308     1.06
    2     89      93     2.98
    4     46      40    -0.38
    6    242     237    -2.61
    8    -25      17     2.44
   -8    113     122     0.27
   -6    249     248    -3.12
   -4    415     424     0.42
   -2    482     470     2.71

 H=    5,  K=    2

    1    192     184    -0.83
    3    254     232     1.92
    5    -22      30    -1.31
    7     73      74     3.09
   -7     77      75    -1.63
   -5    167     178     1.75
   -3    178     164     1.18
   -1     93      91     1.24

 H=    6,  K=    2

    0    313     287     0.91
    2    529     543     0.50
    4     90      99     0.57
    6    179     185     0.42
  -11    637      41    -2.09
   -8     43      40    -0.35
   -6    237     237    -0.25
   -4    303     300    -2.88
   -2    914     943     0.09

 H=    7,  K=    2

    1     69      74     0.45
    3    108     100    -1.35
    5    223     218     1.94
    7    -24      27     0.96
   -7    197     203     1.90
   -5    -21      26    -1.87
   -3    162     174     1.90
   -1    119     124    -0.44

 H=    8,  K=    2

    0    596     565    -0.15
    2    107     114    -2.75
    4    138     141    -0.21
    6     88      88    -2.04
   -8     58      57    -1.95
   -6    171     167    -2.86
   -4    133     128    -1.79
   -2    712     710    -3.01

 H=    9,  K=    2

    1    384     378    -1.05
    3    115     114    -0.65
    5    148     145    -1.37
   -7    140     148    -1.75
   -5    316     312     1.99
   -3    100     105    -1.80
   -1    172     153    -1.63

 H=   10,  K=    2
```

```
    L     FO      FC    ALPHA

    0    626     632     2.90
    2    236     231    -0.02
    4    168     178    -2.94
    6    -25      21    -1.85
   -8     99      92     2.69
   -6     49      70    -2.89
   -4    294     287    -3.06
   -2     64      47    -2.84

 H=   11,  K=    2

    1    -21      21    -2.16
    3    150     154    -1.37
    5     43      31     2.55
   -7     84      84    -1.43
   -5     92      91    -2.07
   -3    535     530     1.84
   -1     40      19     2.42

 H=   12,  K=    2

    0    277     278     0.32
    2    291     289     2.24
    4    215     215     0.21
   -6     58      41    -0.75
   -4     66      60    -1.38
   -2    126     121    -2.83

 H=   13,  K=    2

    1     64      62     0.13
    3     38      42     1.68
    5     59      58    -1.90
   -7     61      75    -0.88
   -5     66      57    -2.55
   -3     86      76    -2.45
   -1    428     411     1.65

 H=   14,  K=    2

    0    197     193    -2.70
    2    173     172    -0.18
    4     92      87     2.79
   -6    245     247    -0.05
   -4    140     147    -1.86
   -2    127     135    -2.31

 H=   15,  K=    2

    1    198     188     0.96
    3    119     115    -0.54
   -5    118     112    -1.46
   -3    121     118    -3.14
   -1    129     123    -1.48

 H=   16,  K=    2

    0     89      92     2.59
    2    170     173     3.05
   -6     91      93     2.54
   -4    229     238     0.02
   -2    119     123    -2.13

 H=   17,  K=    2

    1     56      46    -1.24
   -5    -26      17     2.72
   -3     88      87    -2.62
   -1    180     188     2.52

 H=   18,  K=    2

    0     40      33    -1.10
   -4     56      59     2.98
   -2    237     245    -0.04

 H=   19,  K=    2

   -3     47      58     2.98
   -1     69      73    -2.68
   L    FO     FC   ALPHA

H=    0,  K=    3

   1   147    141   -2.83
   3   516    513   -1.84
   5   153    160    2.29
   7   144    146   -1.98

H=    1,  K=    3

   0   597    559   -2.89
   2   210    165   -2.03
   4   493    494   -3.03
   6   156    156   -0.24
   8    89     94   -2.54
  -8   155    148    2.22
  -6    93     83    0.47
  -4   312    309    2.96
  -2   550    538   -0.02

H=    2,  K=    3

   1   275    230    1.23
   3   265    250    1.55
   5   118    115   -1.97
   7   151    157    1.86
  -7   149    148   -0.97
  -5   303    294    1.43
  -3    61     67   -1.02
  -1   829    819    1.42

H=    3,  K=    3

   0   709    703   -0.09
   2   449    435   -2.96
   4    81     86   -0.26
   6   188    183    2.85
   8    97    105    0.04
  -8    39     44   -0.53
  -6   163    160    1.83
  -4   432    438    0.12
  -2   116    128    1.12

H=    4,  K=    3

   1   318    304    0.61
   3   181    204   -0.89
   5    92     99    0.81
   7   103    101   -1.06
  -7   -23     27    2.20
  -5   397    395   -1.53
  -3   278    282    1.51
  -1   329    310   -1.30

H=    5,  K=    3

   0   163    161    0.45
   2   447    451   -0.20
   4   168    165    3.09
   6   159    165    0.45
  -8   176    172   -2.85
  -6    72     66   -1.43
  -4   172    161    0.93
  -2   815    836    0.12

H=    6,  K=    3

   1   212    176   -1.91
   3   -19     16    0.49
   5   145    145   -1.90
   7    59     52    2.60
  -7    60     60   -2.26
  -5   181    177    1.95
  -3   467    448   -1.92
  -1   513    517    1.80

H=    7,  K=    3

   0   319    312    0.0
   2   405    402   -2.71
```

```
   L    FO     FC   ALPHA

   4   173    173   -1.42
   6   168    175   -2.65
  -8   -24     24   -0.36
  -6   427    441   -3.14
  -4   224    209   -3.11
  -2   158    154    2.27

H=    8,  K=    3

   1   472    486    1.52
   3   -21     17    0.35
   5    70     76    1.65
   7    55     50   -2.73
  -7    77     82    0.30
  -5    64     78   -1.18
  -3   333    327    1.44
  -1   306    279   -1.85

H=    9,  K=    3

   0    77     77    1.67
   2   184    184   -0.13
   4   232    236   -2.78
   6    46     39   -1.16
  -8    57     53   -3.13
  -6   115    113   -0.32
  -4   388    391    3.01
  -2   175    173    1.35

H=   10,  K=    3

   1   319    328   -1.42
   3   189    187    0.82
   5   111    112   -0.59
  -7   100     94   -1.77
  -5   137    140   -1.06
  -3   266    296   -1.62
  -1   187    190    1.11

H=   11,  K=    3

   0   363    366    0.74
   2    53     43   -0.32
   4   172    171    0.08
   6    62     65    2.93
  -6    63     69   -2.48
  -4   288    276   -0.20
  -2   208    200    2.15

H=   12,  K=    3

   1   172    168    1.84
   3   180    180   -1.81
   5   -25     34    1.35
  -7   198    199    1.73
  -5    80     89    2.64
  -3    87     87   -2.39
  -1   303    307   -2.23

H=   13,  K=    3

   0   183    189    2.52
   2   111    116    0.36
   4   154    156   -2.00
  -6    93     96   -0.95
  -4   214    204   -2.91
  -2   195    187   -0.03

H=   14,  K=    3

   1   136    149   -2.57
   3   177    175    1.70
  -5   251    257    1.43
  -3   174    192    1.61
  -1   100     97    2.07

H=   15,  K=    3

   0   212    209    0.47
   2   111    114    2.41
```

```
   L    FO     FC   ALPHA

   4    67     77    0.35
  -6   180    173   -3.02
  -4    73     76   -0.94
  -2   155    156    2.72

H=   16,  K=    3

   1    55     48    0.69
   3    87     89   -1.54
  -5   261    263   -1.36
  -3   111    112    0.94
  -1   110    111    0.85

H=   17,  K=    3

   0   125    128    2.07
   2   176    173    0.41
  -4   188    192   -2.82
  -2    51     68    0.10

H=   18,  K=    3

   1   -25     26    0.99
  -3   251    255   -1.66
  -1   -25     34    2.95

H=   19,  K=    3

   0   -25      8    2.18
  -2   241    233   -2.86

H=    0,  K=    4

   0    66    112   -3.14
   2   298    270    0.05
   4   191    181    0.46
   6   117    113   -0.02
   8    55     56    1.19

H=    1,  K=    4

   1   242    249   -1.43
   3   409    395    1.84
   5    89     92   -2.43
   7   273    274    1.60
  -7    52     56   -2.26
  -5   518    522    1.43
  -3   273    280   -0.96
  -1   163    148    0.13

H=    2,  K=    4

   0   192    191   -1.64
   2   179    190   -2.66
   4   147    163   -0.98
   6    82     81   -0.24
   8    71     69   -0.93
  -8    76     70    2.93
  -6   111    112   -2.66
  -4    64     61   -0.14
  -2   164    156   -2.23

H=    3,  K=    4

   1   605    596   -1.40
   3   427    440   -1.50
   5   161    159    1.66
   7   158    153   -1.29
  -7    38     31   -2.84
  -5   194    191   -2.15
  -3   523    530    1.50
  -1   882    888   -1.40

H=    4,  K=    4

   0   340    322    2.71
   2   148    141    2.92
   4   158    157    2.52
   6    60     59   -2.75
  -8   -25     26    2.22
```

```
   L     FO      FC   ALPHA

  -6     78      79    2.09
  -4    198     194    2.47
  -2    121     145    1.22

H=    5,  K=     4

   1    481     481   -1.44
   3    146     146   -2.64
   5    185     188   -2.25
   7    158     153    1.99
  -7     79      78   -1.85
  -5    237     239    1.58
  -3     53      40    2.75
  -1    758     751    1.46

H=    6,  K=     4

   0    151     127   -0.60
   2     86      96    2.26
   4     40      32    1.56
   6     93      89    1.41
  -8     45      52   -0.55
  -6     46      51   -0.83
  -4     88      85   -0.37
  -2    133     133    2.22

H=    7,  K=     4

   1    496     498    1.20
   3    170     180   -1.46
   5    149     149    2.37
   7     72      73   -2.43
  -7    103      92    1.59
  -5     59      58   -1.85
  -3    322     340    1.49
  -1    237     238   -0.90

H=    8,  K=     4

   0    115     114   -2.92
   2    227     233   -1.55
   4     38      47   -1.54
   6     34      36   -1.55
  -8     45      47   -2.25
  -6     71      72   -1.23
  -4     53      63   -0.85
  -2    167     169   -1.17

H=    9,  K=     4

   1    562     568   -1.07
   3    188     191    0.48
   5    163     167   -1.25
  -7    173     169   -1.85
  -5    142     134    2.37
  -3    214     206   -1.90
  -1     90     103    0.78

H=   10,  K=     4

   0     43      53   -1.22
   2    122     117    2.24
   4     94      98   -2.28
   6    -26      31    2.99
  -6     55      62    2.50
  -4     67      63    0.67
  -2    173     180    0.88

H=   11,  K=     4

   1    189     193    1.59
   3    234     236   -1.35
   5     96      96    1.94
  -7    138     144    1.69
  -5    103     100    3.09
  -3    419     412    2.01
  -1     75      77   -2.54

H=   12,  K=     4
```

```
   L     FC      FC   ALPHA

   0    207     211    0.46
   2     77      87   -0.54
   4    101     108    1.12
  -6    -24      14   -1.05
  -4     68      62    2.44
  -2     75      78    0.55

H=   13,  K=     4

   1    101     100   -0.60
   3    154     154    1.56
   5     84      89   -1.64
  -7    232     229   -1.37
  -5    138     148    1.79
  -3    108     111    2.69
  -1    381     377    1.71

H=   14,  K=     4

   0     89      80   -2.49
   2    105     107   -0.39
   4     98      97   -1.23
  -6     57      57   -0.05
  -4     80      83   -2.03
  -2    125     135    3.05

H=   15,  K=     4

   1    193     188    0.97
   3    206     211   -0.76
  -5    351     354   -1.56
  -3     86      90    3.03
  -1    130     121   -1.75

H=   16,  K=     4

   0    163     167    2.64
   2    124     122    3.13
  -4     79      80    0.46
  -2     51      44   -3.07

H=   17,  K=     4

   1     71      82   -2.17
  -3    229     242   -2.05
  -1    170     167    2.68

H=   18,  K=     4

   0     40      37    0.06
  -2    125     130    0.27

H=    0,  K=     5

   1    288     281    2.21
   3    195     198    2.07
   5     88      77   -2.47
   7    -23      14   -1.55

H=    1,  K=     5

   0    688     668   -2.89
   2    230     220   -1.56
   4    461     468   -2.98
   6    195     187   -0.44
  -8    183     181    2.84
  -6    133     126    1.21
  -4    554     541   -3.14
  -2    145     139   -0.37

H=    2,  K=     5

   1    184     183   -1.26
   3    137     145    1.84
   5    112     115    1.19
   7    -24      11   -0.64
  -7    -23      32    0.04
  -5    132     131   -0.79
  -3     61      78   -0.90
  -1    214     206   -1.08
```

```
   L     FO      FC   ALPHA

H=    3,  K=     5

   0    135     134    0.31
   2    517     509    3.13
   4     99      86   -0.35
   6    268     270    2.88
  -8    107     110    0.35
  -6    152     155    2.55
  -4    458     456    0.43
  -2    508     486    2.99

H=    4,  K=     5

   1     60      73   -0.15
   3    106      99   -1.24
   5    -22       4    1.19
   7     63      66    0.41
  -7     57      58    1.06
  -5    -22      28   -0.16
  -3    333     322   -1.28
  -1    149     146   -1.08

H=    5,  K=     5

   0    263     250   -3.14
   2    232     223   -0.17
   4    176     174    2.90
   6    211     204    0.11
  -8    125     122   -2.38
  -6    209     210   -0.06
  -4    -20      11    0.76
  -2    908     889    0.07

H=    6,  K=     5

   1    154     130   -2.86
   3    132     139    2.58
   5     88      78   -2.20
   7     58      60   -2.28
  -7     81      80    2.45
  -5    156     156    1.80
  -3    109      94    2.53
  -1    359     342   -1.81

H=    7,  K=     5

   0    586     576   -0.17
   2    441     441   -2.80
   4    144     146   -1.67
   6    169     165   -2.91
  -8    -24       7    2.06
  -6    324     316   -3.06
  -4    173     175    0.43
  -2    163     172    3.06

H=    8,  K=     5

   1    133     130   -1.52
   3     93      92    2.12
   5    103     115    1.76
  -7     66      59    0.72
  -5     55      60    1.41
  -3    179     168    0.89
  -1    188     172    0.86

H=    9,  K=     5

   0    144     145    2.20
   2    404     404   -0.11
   4    232     222   -3.10
   6    -25      12   -2.35
  -6     57      55    0.89
  -4    318     313    2.82
  -2    447     447    0.51

H=   10,  K=     5

   1    160     158    0.62
   3     65      64   -1.99
   L     FO      FC    ALPHA

   5     39      35     1.71
  -7     39      48     2.42
  -5     44      44     0.41
  -3     72      67    -0.65
  -1    155     157    -0.05

 H=   11,  K=     5

   0    467     472     0.30
   2     48      52     1.73
   4    289     285    -0.08
  -6    205     210    -2.67
  -4    119     114     0.11
  -2    222     214     2.53

 H=   12,  K=     5

   1     91      86    -1.37
   3    -24       3     1.23
   5     98      98    -2.44
  -7     61      60    -2.43
  -5    108     109     2.64
  -3     62      53    -2.36
  -1    117     106    -1.61

 H=   13,  K=     5

   0    304     293     3.09
   2    170     164    -0.44
   4    143     140    -2.52
  -6    125     133    -0.64
  -4    352     361    -2.90
  -2    -24      20    -0.08

 H=   14,  K=     5

   1     41      49    -0.54
   3    -26      13    -1.40
  -5    -25      24     3.14
  -3     56      51     1.45
  -1     56      50    -0.53

 H=   15,  K=     5

   0    159     149     0.60
   2    192     184     2.91
  -4    140     143    -0.23
  -2    240     241     2.79

 H=   16,  K=     5

   1     49      56    -0.44
  -5     45      49     2.01
  -3    -25      21     2.36
  -1     82      87     0.20

 H=   17,  K=     5

   0    139     142     1.95
  -4    183     186    -2.76
  -2    180     177     0.09

 H=   18,  K=     5

  -3     88      86     2.65
  -1     42      41     2.65

 H=    0,  K=     6

   0     44      23     0.0
   2    212     211     2.69
   4    180     179     2.79
   6    115     118     0.30

 H=    1,  K=     6

   1    826     820    -1.56
   3    415     404     1.57
   5     80      93    -1.81
   7    200     195     1.49
```

```
   L     FO      FC    ALPHA

  -7    126     122    -1.26
  -5    301     297     1.32
  -3    308     322    -1.02
  -1    455     431     1.06

 H=    2,  K=     6

   0    399     396    -2.66
   2    187     183    -0.87
   4    101      92     0.35
   6     45      53    -2.95
  -6     55      36    -1.45
  -4    298     296    -0.39
  -2    298     303    -2.55

 H=    3,  K=     6

   1    175     153     0.69
   3    685     687    -1.67
   5    147     146     1.09
   7    135     139    -1.24
  -7    118     120     2.09
  -5    237     231    -1.88
  -3    309     294     1.57
  -1    628     622    -1.47

 H=    4,  K=     6

   0    259     258    -3.05
   2    285     275     2.92
   4     66      63     0.45
   6    114     109     0.84
  -6    129     125     0.42
  -4     71      65     0.79
  -2    380     359     0.07

 H=    5,  K=     6

   1    289     282    -1.97
   3    304     310     1.83
   5    305     298    -2.21
   7    105     105     1.81
  -7    121     117    -1.90
  -5    362     363     1.72
  -3     79      96    -3.03
  -1    620     611     1.57

 H=    6,  K=     6

   0    241     229    -0.42
   2    150     157    -2.48
   4    119     117     2.62
   6    -24      13    -0.02
  -6     56      57     1.20
  -4    161     159     0.18
  -2    136     129    -2.98

 H=    7,  K=     6

   1    529     518     1.24
   3     90      81    -1.67
   5    248     257     1.59
  -7    151     151     1.36
  -5    212     205    -1.51
  -3    394     393     1.33
  -1    153     147    -0.69

 H=    8,  K=     6

   0    276     277    -2.71
   2    196     197    -0.71
   4     53      72    -1.40
   6    -25      37     1.58
  -6    -24      20     1.81
  -4     87      86     0.27
  -2    149     140    -0.26

 H=    9,  K=     6

   1    424     425    -1.27
```

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   L     FO      FC    ALPHA

   3    174     177     0.65
   5    165     161    -1.23
  -7    247     245    -1.70
  -5    135     139     1.83
  -3    399     390    -1.71
  -1    127     138     0.51

 H=   10,  K=     6

   0    -22      10     2.09
   2    274     272     3.12
   4    -25      41     0.16
  -6     63      61     1.94
  -4    142     145     0.99
  -2     87      87     1.09

 H=   11,  K=     6

   1    104     109     1.68
   3    265     263    -1.86
   5     73      71     2.11
  -7    167     163     1.61
  -5    206     211    -2.05
  -3    373     362     1.83
  -1    222     212    -2.10

 H=   12,  K=     6

   0     78      74    -1.89
   2     65      64    -1.88
   4    152     148     3.00
  -6    -25      18    -2.41
  -4     96      96     0.69
  -2    158     161     0.42

 H=   13,  K=     6

   1     66      62    -0.84
   3    145     140     1.36
  -5    217     220     1.33
  -3    162     166    -1.88
  -1    388     383     1.45

 H=   14,  K=     6

   0    180     181    -0.18
   2    118     119    -1.57
  -4     41      32     0.95
  -2    149     151     0.27

 H=   15,  K=     6

   1    197     200     0.97
   3    136     137    -0.76
  -5    206     201    -1.73
  -3    132     135     1.36
  -1    228     231    -1.68

 H=   16,  K=     6

   0     78      79     0.55
   2     95     100    -0.17
  -4    110     114     2.57
  -2    122     122     1.61

 H=   17,  K=     6

   1    159     154    -2.19
  -3    172     181    -2.37
  -1    180     176     1.86

 H=    0,  K=     7

   1    179     176     2.47
   3    342     341     1.79
   5    175     174    -1.75
   7    -24      26     0.67
  L    FO     FC   ALPHA

H=    1,  K=    7

  0   486    475   -2.85
  2   147    152   -0.80
  4   165    170   -2.30
  6    59     67   -1.05
 -6    77     76    0.86
 -4   151    147    3.01
 -2   100    110   -2.10

H=    2,  K=    7

  1    95     96    2.51
  3   119    115    1.20
  5   193    192    1.32
  7    98    102   -1.35
 -7   113    113    1.39
 -5   155    156   -1.04
 -3   168    153    1.35
 -1   362    362   -1.62

H=    3,  K=    7

  0   197    189    0.68
  2   354    346    2.88
  4   132    135    1.18
  6    85     87    2.87
 -6    92     90    2.79
 -4   278    233    0.65
 -2   135    141    1.54

H=    4,  K=    7

  1    91     84   -2.61
  3   237    240    2.02
  5    89     86    0.86
 -7    37     34   -1.28
 -5   190    190    1.17
 -3   308    312   -1.21
 -1   269    252    1.37

H=    5,  K=    7

  0   137    120   -0.59
  2   323    326    0.04
  4    93     95    2.87
  6   146    143    0.57
 -6   159    152   -0.29
 -4   139    141   -2.49
 -2   352    332   -0.05

H=    6,  K=    7

  1   184    185    2.07
  3   127    129   -2.90
  5   127    118    2.36
 -7   156    149    1.82
 -5    88     89   -1.97
 -3    80     74    0.42
 -1   539    538   -1.59

H=    7,  K=    7

  0   169    177   -0.89
  2   219    224   -2.30
  4   121    125   -0.58
  6   125    121   -2.60
 -6   275    280   -3.03
 -4   -23     10   -2.82
 -2   364    364   -2.89

H=    8,  K=    7

  1   463    460   -1.64
  3   119    119    1.90
  5   -24     20   -1.76
 -7    51     56   -1.85
 -5   208    209    1.45
 -3   202    194   -1.22
```

```
  L    FO     FC   ALPHA

 -1   211    216   -0.50

H=    9,  K=    7

  0   284    281    2.81
  2   113    116    0.03
  4   159    157   -3.14
 -6   201    200    0.43
 -4   248    249    2.81
 -2   154    147    1.25

H=   10,  K=    7

  1    91     87    0.07
  3   236    239   -2.09
  5   108    106    1.96
 -5   -24     18    2.73
 -3   302    298    1.26
 -1   153    157   -0.75

H=   11,  K=    7

  0   183    178    0.17
  2    64     85    2.44
  4   177    176   -0.07
 -6    59     51   -1.68
 -4   337    339    0.09
 -2    83     89   -3.11

H=   12,  K=    7

  1    90     92   -1.01
  3   -25     13    2.80
 -5    91    100    2.11
 -3    44     43   -2.05
 -1   223    220    1.08

H=   13,  K=    7

  0   151    156   -2.56
  2   109    100   -0.87
 -4   186    173   -2.83
 -2   225    226   -0.03

H=   14,  K=    7

  1   165    163    0.85
  3   -27     42   -0.56
 -5    59     65   -2.97
 -3    51     58    1.69
 -1   129    127   -0.81

H=   15,  K=    7

  0   171    173    0.48
  2    96     90    3.00
 -4    64     67    1.05
 -2   203    203    2.85

H=   16,  K=    7

  1    55    105   -0.96
 -3    52     35    3.02
 -1    44     54    1.09

H=   17,  K=    7

 -2   116    114    0.22

H=    0,  K=    8

  0   541    530    3.14
  2    64     58    1.12
  4   124    118    2.58
  6   102    107   -0.30

H=    1,  K=    8

  1   139    141    0.35
  3   218    222    1.26
```

```
  L    FO     FC   ALPHA

  5   -24     46    0.48
  7   153    151    1.28
 -7   163    162   -0.80
 -5   116    123    1.11
 -3   131    141   -0.30
 -1   340    340    1.11

H=    2,  K=    8

  0   134    130   -0.33
  2   289    296    3.08
  4   165    166    0.49
  6    43     55    1.93
 -6    85     82    0.59
 -4   224    216   -0.11
 -2   172    167   -2.33

H=    3,  K=    8

  1   134    138    1.43
  3   187    192   -1.08
  5    49     57   -0.53
 -7    67     65    2.84
 -5   327    318   -1.47
 -3    49     38    2.68
 -1   206    188   -1.52

H=    4,  K=    8

  0   277    265   -2.86
  2   147    147    0.38
  4   148    154    2.66
  6   118    120    0.54
 -6    43     41   -0.67
 -4   136    141    0.10
 -2   187    178   -0.07

H=    5,  K=    8

  1   185    180   -2.67
  3   189    186    2.31
  5   104    110   -1.86
 -7    60     61   -2.02
 -5   153    144    2.07
 -3   346    337   -1.72
 -1   199    210    2.24

H=    6,  K=    8

  0    97     88   -1.42
  2   350    349   -2.87
  4    80     75    0.25
  6    92     87   -3.11
 -6   149    147    2.82
 -4   -23     26   -2.80
 -2    91    103   -1.31

H=    7,  K=    8

  1   219    222    1.29
  3   -23     23   -0.02
  5   157    155    1.52
 -5   115    118   -0.98
 -3   204    195    0.82
 -1   308    307   -1.36

H=    8,  K=    8

  0   150    160   -1.44
  2   113    113   -0.37
  4   160    156   -3.14
 -6   239    248    0.27
 -4   -24     36    2.20
 -2   -23     15   -0.33

H=    9,  K=    8

  1   323    318   -1.74
  3    74     78    0.58
  5    96    102   -0.91
```

```
   L     FO      FC    ALPHA

  -5    149     148     1.76
  -3    148     148    -1.57
  -1    121     120     0.66

 H=   10, K=      8

   0     36      44     2.62
   2    120     113    -2.12
   4     97      97     0.35
  -6     96     110     2.86
  -4    374     384     0.30
  -2    -23      15     0.78

 H=   11, K=      8

   1    151     145     1.95
   3    243     238    -2.43
  -5     75      71    -2.36
  -3    235     241     1.88
  -1    103     107     3.14

 H=   12, K=      8

   0    114     114    -2.03
   2     71      78    -2.90
  -4    175     185     2.79
  -2    322     326     0.16

 H=   13, K=      8

   1     72      71     1.59
   3    165     157     1.38
  -5     63      50     0.62
  -3    150     137    -0.83
  -1    211     214     1.24

 H=   14, K=      8

   0    282     273    -0.04
   2     91      91    -1.74
  -4    102     105     0.84
  -2    133     146     2.61

 H=   15, K=      8

   1     61      59     0.29
  -3    -27      48    -0.88
  -1    226     221    -1.11

 H=   16, K=      8

   0    107     111     2.78
  -2    137     148     0.70

 H=    0, K=      9

   1    337     329    -1.73
   3    253     248     1.56
   5    108     118    -1.31

 H=    1, K=      9

   0    123     126    -2.67
   2     67      72    -1.01
   4     72      71    -2.44
   6    112     110    -0.68
  -6    -24      40    -2.23
  -4    239     242    -3.05
  -2     71      79    -2.87

 H=    2, K=      9

   1    318     310     1.76
   3    281     285    -1.63
   5     83      80     0.99
  -5    185     184    -1.74
  -3     32      28     1.40
  -1    440     422    -1.71

 H=    3, K=      9
```

```
   L     FO      FC    ALPHA


   0    159     152     1.54
   2    155     157     1.80
   4    100      94     1.54
   6    111     113     2.62
  -6    107     109     0.73
  -4     94     101     0.84
  -2    234     242     2.56

 H=    4, K=      9

   1    252     253    -2.03
   3    363     367     1.76
   5     92      97    -1.89
  -5    156     159    -0.03
  -3    151     152    -1.44
  -1    156     156     1.74

 H=    5, K=      9

   0     70      71    -2.29
   2    141     138     0.05
   4     76      74     0.39
  -6    124     122    -1.39
  -4     78      87    -0.96
  -2    136     134    -0.68

 H=    6, K=      9

   1    163     170     1.82
   3    171     172    -1.91
   5    206     207     1.59
  -5    -24      17     1.75
  -3    171     176    -0.69
  -1    214     217    -1.36

 H=    7, K=      9

   0     87      93    -1.41
   2     86      84    -2.14
   4     66      64    -0.61
  -6    -25      18    -2.96
  -4    156     157    -2.30
  -2    175     165    -2.43

 H=    8, K=      9

   1    199     201    -1.38
   3    119     130     1.74
   5    132     128    -1.55
  -5    271     282     1.60
  -3     44      50    -0.26
  -1    165     171    -1.36

 H=    9, K=      9

   0    158     148     2.84
   2    102     107     1.63
   4     81      85     2.31
  -6    146     140     0.63
  -4    101      95     1.30
  -2    129     135     2.92

 H=   10, K=      9

   1    116     113    -3.00
   3     71      70    -1.89
  -5    159     162    -1.66
  -3    309     320     1.46
  -1     82      81     0.40

 H=   11, K=      9

   0     49      52    -2.13
   2    -25      18    -2.02
  -4    149     144    -0.15
  -2     77      72    -0.78

 H=   12, K=      9
```

```
   L     FO      FC    ALPHA

   1    111     108    -0.53
   3    113     107     2.97
  -5    134     137     1.57
  -3    265     272    -1.43
  -1    170     169     1.07

 H=   13, K=      9

   0    112     117    -1.82
   2     59      57    -2.20
  -4     50      40    -2.76
  -2     98      94    -1.20

 H=   14, K=      9

   1     58      55     0.39
  -3    162     164     1.35
  -1    300     297    -1.37

 H=   15, K=      9

  -2     69      69     2.39

 H=    0, K=     10

   0    396     393     3.14
   2     42      39     1.49
   4    194     199     3.05
   6    209     207    -0.33

 H=    1, K=     10

   1    338     338     1.23
   3    126     132    -0.06
   5    107     113    -0.85
  -5    132     132    -0.98
  -3    128     131    -1.28
  -1     59      59    -0.57

 H=    2, K=     10

   0    132     134     0.18
   2    245     242     2.86
   4    113     116     0.83
  -6     65      57     2.49
  -4    403     406     0.07
  -2    120     127    -2.91

 H=    3, K=     10

   1     92      89    -1.99
   3    140     137     1.11
   5     93      92    -0.46
  -5    106     110     2.16
  -3    113     110    -2.11
  -1     81      79    -2.80

 H=    4, K=     10

   0    164     162    -2.68
   2    162     160     0.07
   4    102     101     3.06
  -6     70      66    -0.32
  -4    127     122    -2.95
  -2    434     443    -0.21

 H=    5, K=     10

   1    199     206     2.49
   3    115     122    -2.57
   5    -25      43     2.20
  -5    154     152    -1.51
  -3    204     203     1.97
  -1    200     212     2.78

 H=    6, K=     10

   0    261     266    -0.43
   2    240     238    -3.04
   4     71      69     0.10
   L     FO     FC   ALPHA

  -4     44     45    0.42
  -2    272    274   -3.06

 H=    7, K=   10

   1    155    160    1.84
   3    159    161    1.38
  -5    105    114    0.62
  -3    259    254   -1.23
  -1    234    238    1.07

 H=    8, K=   10

   0    195    208    3.03
   2    188    187   -0.09
   4    145    149    2.66
  -4    143    139    2.89
  -2    169    167    0.19

 H=    9, K=   10

   1    102    107    0.88
   3     38     40    2.43
  -5    141    141   -1.46
  -3     68     81   -0.54
  -1    285    282   -1.84

 H=   10, K=   10

   0    198    196   -0.22
   2    135    142   -3.08
  -4    236    238    0.11
  -2    109    108   -2.91

 H=   11, K=   10

   1    263    269   -2.51
  -3    146    152   -1.74
  -1     45     44   -2.09

 H=   12, K=   10

   0    159    156   -2.77
   2    108    111   -0.62
  -4    190    180    3.11
  -2    172    174   -0.05

 H=   13, K=   10

   1     58     56    0.76
  -3    119    117    0.19
  -1     78     76   -0.87

 H=    0, K=   11

   1     93     75   -0.71
   3    124    125    0.97
   5    202    197   -1.50

 H=    1, K=   11

   0    156    156    0.02
   2     79     86   -3.06
   4     51     55   -1.78
  -4    164    161   -2.68
  -2     78     76   -2.70

 H=    2, K=   11

   1     72     67    3.00
   3    109    105   -1.32
   5     61     59    1.21
  -5    225    224   -1.62
  -3    295    293    1.78
  -1     97     95   -1.91

 H=    3, K=   11

   0    140    142    2.05
   2    228    241    0.52
```

```
   L     FO     FC   ALPHA

   4     91     91    2.13
  -4     96     97    2.66
  -2    243    240    2.76

 H=    4, K=   11

   1     45     44    2.60
   3    142    151    2.28
  -5    181    183    1.64
  -3    254    249   -1.61
  -1    380    394    1.70

 H=    5, K=   11

   0    188    182    2.89
   2    -24     35    1.51
   4    225    220   -0.04
  -4    124    124   -0.55
  -2    151    153   -2.58

 H=    6, K=   11

   1    250    243    1.30
   3     80     76   -0.25
  -5    190    183   -1.13
  -3    184    187    1.22
  -1    360    361   -1.50

 H=    7, K=   11

   0    139    148   -2.68
   2    135    128    2.51
  -4     77     75   -1.47
  -2    121    115   -1.06

 H=    8, K=   11

   1    386    383   -1.76
   3     75     66    0.90
  -3    240    242   -1.55
  -1    153    152    1.60

 H=    9, K=   11

   0     52     34    0.08
   2    121    121    2.56
  -4     65     80    0.55
  -2     40     36   -2.64

 H=   10, K=   11

   1    219    222    1.73
  -3    191    185    1.67
  -1    161    156   -1.92

 H=   11, K=   11

   0     87     85   -1.84
  -2     82     91   -0.87

 H=   12, K=   11

  -1    191    187    1.27

 H=    0, K=   12

   0    144    136    3.14
   2     85     87   -0.47
   4    235    237   -3.02

 H=    1, K=   12

   1    396    407    1.34
   3     58     71   -0.45
  -3    -24     26    0.84
  -1     59     57   -1.13

 H=    2, K=   12

   0    209    209    0.56
```

```
   L     FO     FC   ALPHA

   2    107    109    2.18
   4    109    109    0.37
  -4    177    184    0.21
  -2    168    177    2.68

 H=    3, K=   12

   1    105    116   -1.81
   3    251    258    1.16
  -3    181    182   -1.88
  -1     51     55   -3.13

 H=    4, K=   12

   0     96    100   -2.74
   2    185    183   -0.11
  -4    152    158   -2.82
  -2    242    247   -0.37

 H=    5, K=   12

   1     97     99   -3.07
   3    157    164   -2.02
  -3    125    117    2.15
  -1    146    151   -2.28

 H=    6, K=   12

   0    161    164   -0.26
   2    126    130   -3.00
  -4     49     49    0.0
  -2    233    241    3.11

 H=    7, K=   12

   1    -24     25   -0.12
  -3    122    119   -1.29
  -1    173    179    1.60

 H=    8, K=   12

   0    199    197    2.60
   2    147    148    0.34
  -2    126    135    0.39

 H=    9, K=   12

   1    172    177    1.81
  -1    120    121   -1.90

 H=   10, K=   12

   0    145    152   -0.16
  -2    107    107   -2.64

 H=   15, K=   12

  15      0      0    0.96

 H=    0, K=   13

   1    152    152   -0.95
   3    161    166    0.85

 H=    1, K=   13

   0    168    174    0.22
   2    108    114    2.82
  -2    104    103    3.01

 H=    2, K=   13

   1    -24     17    1.62
   3    193    200   -1.72
  -3     61     62    2.61
  -1    187    188   -1.62

 H=    3, K=   13

   0    103    102    2.36
   L     FO      FC    ALPHA       L     FO      FC    ALPHA       L     FO      FC    ALPHA

   2    182     190     0.23       0     60      61     0.11       0    222     228    -3.09
  -2     96      89     0.18       2     47      39     2.60
                                  -2    234     235    -2.92     H=     0,  K=   14
 H=     4,  K=   13
                                 H=     6,  K=   13                0     50      58     3.14
   1    117     120    -1.80
  -3     65      68     2.22       1    154     158     1.00     H=     1,  K=   14
  -1    146     152     1.86      -1     68      73     0.54
                                                                  -1     64      62    -1.80
 H=     5,  K=   13              H=     7,  K=   13
```

```
   L    FC       FC   ALPHA

 H=     0,  K=     0

   2   159      99    2.71
   4   233     252    0.16
   6   223     220    2.71
   8   215     221    0.46

 H=     2,  K=     0

   0   974    1080    3.11
   2  1899    2437   -0.19
   4   460     462   -2.86
   6   124     120   -1.35
   8   146     144   -2.95
  -8   215     212   -3.11
  -6    36      50   -0.57
  -4   781     760    3.13
  -2   207     168   -3.09

 H=     4,  K=     0

   0   221     237    1.67
   2  1173    1278    2.98
   4   875     858   -0.42
   6   307     320   -3.10
   8    34      26   -2.14
  -8   192     195    0.02
  -6   386     377    2.99
  -4   101      87    2.06
  -2   907     929    2.84

 H=     6,  K=     0

   0   387     403    1.59
   2   595     580    0.39
   4   575     588    2.80
   6   431     423   -0.30
   8   126     130    2.18
  -8    89      83   -2.59
  -6   437     429   -0.32
  -4   346     365   -2.97
  -2   413     428    0.13

 H=     8,  K=     0

   0   309     299    0.02
   2   124     117    2.98
   4   273     289   -0.54
   6   314     315   -3.04
   8   206     212   -0.81
  -8   237     233    0.03
  -6   347     348   -3.01
  -4   276     282   -0.92
  -2   652     659   -2.98

 H=    10,  K=     0

   0   494     463    2.68
   2   290     300    0.53
   4   121     111   -2.94
   6   125     134   -0.73
  -8   189     190    3.06
  -6   386     387    0.07
  -4   514     510   -3.08
  -2   168     173   -0.59

 H=    12,  K=     0

   0   365     385    0.37
   2   326     338    1.83
   4   316     330    0.60
   6   -25      48    1.46
  -8   274     272    0.13
  -6   209     213   -3.13
  -4   599     591   -0.19
  -2   312     292   -3.00

 H=    14,  K=     0
```

```
   L    FO       FC   ALPHA

   0   365     355   -2.84
   2   128     136   -0.05
   4   117     117    2.97
   6   128     133   -0.13
  -8   138     132    2.98
  -6   223     222   -0.17
  -4   525     529   -2.91
  -2   438     445   -0.75

 H=    16,  K=     0

   0   212     218   -0.68
   2   262     267    3.02
   4    41      37    0.10
  -6   147     151    2.60
  -4   251     256   -0.38
  -2   529     535   -2.98

 H=    18,  K=     0

   0   293     282    2.92
   2   170     165    0.24
  -6   178     175    0.38
  -4    63      66    1.95
  -2   380     378   -0.30

 H=    20,  K=     0

   0   288     290   -0.62
   2   179     178    3.12
  -4    97      93   -0.29
  -2   116     112   -2.49

 H=     0,  K=     1

   1   782     874    1.56
   3   182     203   -1.64
   5   129     122   -3.10
   7   221     222   -2.04
   9    83      80    1.63

 H=     1,  K=     1

   0   185     170   -2.53
   2   492     490    2.95
   4    68      69   -1.97
   6    51      49    0.13
   8   -25      32    2.78
  -8    96      94    3.01
  -6    63      60    1.74
  -4   149     144    2.72
  -2   176     210   -2.93

 H=     2,  K=     1

   1   859     937   -1.46
   3   662     644    1.40
   5   100      87    1.98
   7   223     221    2.09
   9    92      81   -2.58
  -9   106     105    1.09
  -7   176     179   -1.18
  -5   414     413    1.58
  -3   444     431    1.41
  -1   486     484    1.32

 H=     3,  K=     1

   0    92     148   -2.76
   2   448     436   -2.45
   4   307     313    2.72
   6   -23      12   -1.63
   8    47      42    0.23
  -8    41      47   -0.12
  -6   120     119    3.05
  -4   132     123    0.34
  -2    89      85    0.84

 H=     4,  K=     1
```

```
   L    FO       FC   ALPHA

   1   343     341   -0.78
   3  1047    1114   -1.36
   5   218     218    0.57
   7    96     101   -0.67
  -9   173     175   -1.75
  -7    60      68   -2.96
  -5   463     472   -1.67
  -3   310     312    1.91
  -1    89     104   -0.21

 H=     5,  K=     1

   0   277     260    0.11
   2   112     106   -0.04
   4   248     225   -2.18
   6   162     163    2.23
   8   -25      12    0.57
  -8    99      94   -2.96
  -6    98     101   -0.38
  -4   -20      19    1.87
  -2   502     470    0.07

 H=     6,  K=     1

   1    39      56    1.70
   3    77      94    1.14
   5   509     514   -1.68
   7    70      60    1.76
  -9   100      95    1.50
  -7   209     208   -1.76
  -5   232     236    2.29
  -3   271     273   -2.33
  -1   675     717    1.99

 H=     7,  K=     1

   0   398     380   -0.12
   2   147      98   -1.30
   4    88      87   -0.19
   6   139     146   -1.98
   8    69      77    2.24
  -8    71      68   -0.68
  -6   223     214    3.09
  -4    33      47   -0.49
  -2   112     110    1.31

 H=     8,  K=     1

   1   632     655    1.74
   3   117     117    1.00
   5   244     251    1.71
   7   187     189   -2.23
  -9   112     110   -0.62
  -7   168     158    1.00
  -5   222     217   -1.27
  -3   531     541    1.78
  -1   197     191    2.62

 H=     9,  K=     1

   0   159     172    1.32
   2   227     222   -0.25
   4    33      51   -1.96
   6    78      83    0.51
  -8    79      87    0.97
  -6    91      83   -0.64
  -4   257     250    2.99
  -2    60      76    0.94

 H=    10,  K=     1

   1   336     324   -1.30
   3   241     242    0.65
   5   214     214   -0.49
   7   131     129    0.95
  -9    98      96    1.83
  -7   308     305   -1.30
  -5    62      72   -0.73
  -3   425     417   -1.47
  -1   267     274    1.75
  L    FO     FC   ALPHA

H=  11, K=    1

  0    74     80    1.47
  2    87     97    1.80
  4   110    105   -0.35
  6   -25     30   -3.03
 -8   107    104   -2.57
 -6    39     36    1.10
 -4    85     84   -0.40
 -2   207    202    2.59

H=  12, K=    1

  1   293    292    2.06
  3   245    238   -1.63
  5    47     44    1.12
 -7   182    177    1.64
 -5   337    331   -1.44
 -3   201    193    2.34
 -1   277    280   -2.35

H=  13, K=    1

  0   151    148    2.68
  2    40     52   -2.43
  4    55     60   -2.89
  6    57     59   -1.09
 -8   -25     16    0.62
 -6   161    162   -2.68
 -4    61     72   -2.49
 -2    33     26    0.60

H=  14, K=    1

  1   151    154   -3.05
  3   292    279    1.76
  5    80     88   -2.07
 -7   118    116   -0.76
 -5   263    260    1.23
 -3   240    230   -1.49
 -1   369    370    2.15

H=  15, K=    1

  0    94     92    1.15
  2    45     59    2.21
  4    37     29   -1.42
 -6    60     64   -0.15
 -4    76     79   -2.54
 -2   -24     47   -1.72

H=  16, K=    1

  1   139    130    1.70
  3   105    103   -0.74
  5   162    165    0.93
 -7    71     66    0.92
 -5   316    318   -1.06
 -3   147    159    0.67
 -1   338    323   -1.50

H=  17, K=    1

  0   -25     31   -0.76
  2    86     85    1.15
  4   -26     33    1.34
 -6    62     48   -0.50
 -4    89     91   -0.32
 -2    47     52    0.97

H=  18, K=    1

  1   250    241   -2.01
  3    86     84    2.08
 -5    97    102    1.14
 -3   271    266   -1.42
 -1   117    123    2.09

H=  19, K=    1
```

```
  L    FO     FC   ALPHA

  0    73     71    1.20
  2    52     56   -1.53
 -4    68     57   -1.87
 -2   -26     47   -1.23

H=  20, K=    1

  1   177    174    2.18
 -3   147    157    1.18
 -1   187    179   -1.85

H=  21, K=    1

  0   -27     34   -2.62
 -2    40     43   -2.29

H=   0, K=    2

  0   599    572    0.0
  2   168    138   -0.61
  4   192    190    0.39
  6   202    206    2.76
  8   196    196    0.18

H=   1, K=    2

  1   386    410   -1.43
  3    97    106    3.01
  5   152    156    2.61
  7   139    150    1.57
  9   -24      7   -0.36
 -9   -24     13    1.82
 -7   -23     20    0.30
 -5   236    238    1.40
 -3   193    188    0.60
 -1    75     58   -0.41

H=   2, K=    2

  0   138    146   -2.47
  2   201    199   -0.94
  4   374    381   -2.33
  6    77     76   -1.12
  8   121    126   -2.89
 -8   199    201   -2.81
 -6   185    183    0.11
 -4   560    579   -3.11
 -2    96     90   -2.66

H=   3, K=    2

  1   211    174   -0.82
  3   331    342   -1.21
  5    82     85   -2.04
  7    63     61   -1.81
  9    65     67    0.82
 -9   120    119   -1.73
 -7    60     59   -2.95
 -5   -20     19   -0.65
 -3    35     50    1.60
 -1   376    368   -1.17

H=   4, K=    2

  0   326    331    0.96
  2   124    102    2.66
  4    77     78   -0.22
  6   251    251   -2.65
  8   -23     13    2.70
 -8   142    143    0.30
 -6   300    291    3.12
 -4   443    456    0.35
 -2   480    506    2.71

H=   5, K=    2

  1   180    174   -0.97
  3   259    274    1.79
  5   -22     18   -2.75
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```
  L    FO     FC   ALPHA
  7    58     61    3.11
 -9   110    117    1.84
 -7    85     78   -1.50
 -5   146    151    1.86
 -3   175    164    1.21
 -1    74     95    1.40

H=   6, K=    2

  0   301    293    1.08
  2   552    562    0.51
  4    99    105    0.89
  6   206    216    0.43
  8    41     46    2.96
 -8    49     41   -0.74
 -6   268    274   -0.22
 -4   354    345   -2.92
 -2   924    957    0.10

H=   7, K=    2

  1    97     90   -0.05
  3   129    128   -1.41
  5   226    223    2.00
  7   -24     31    1.36
 -9    41     53   -1.75
 -7   213    212    1.35
 -5   -20      1    2.01
 -3   131    146    2.04
 -1   110    118   -0.62

H=   8, K=    2

  0   580    565   -0.12
  2   153    158   -2.88
  4   147    144   -0.40
  6   105    110   -2.17
  8   101    107   -0.11
 -8    46     56   -2.12
 -6   195    200   -2.84
 -4   127    142   -1.42
 -2   761    781   -2.99

H=   9, K=    2

  1   380    389   -0.99
  3   133    141   -0.49
  5   156    160   -1.35
  7    67     72    1.68
 -9   105    100   -1.51
 -7   159    165   -1.82
 -5   310    311    1.99
 -3    48     52   -2.06
 -1   188    170   -1.37

H=  10, K=    2

  0   693    674    2.96
  2   257    269    0.08
  4   194    194   -2.99
  6   -25     32   -1.61
 -8    97     95    2.53
 -6    53     57   -2.96
 -4   314    308   -3.04
 -2   100     50   -0.75

H=  11, K=    2

  1    42     43   -0.73
  3   147    154   -1.34
  5   -24     39    2.47
  7    89     85   -1.95
 -7    81     74   -1.55
 -5   106    101   -2.23
 -3   525    519    1.91
 -1    80     68    2.16

H=  12, K=    2

  0   339    339    0.26
```

L	FO	FC	ALPHA
2	318	314	2.38
4	254	258	0.26
6	52	63	2.38
-8	272	263	0.03
-6	82	66	-0.17
-4	97	93	-0.86
-2	127	128	-2.86
H= 13, K= 2			
1	62	52	0.49
3	38	42	0.80
5	69	71	-1.81
-7	85	86	-0.86
-5	52	51	-3.02
-3	79	90	-2.73
-1	389	386	1.75
H= 14, K= 2			
0	221	228	-2.71
2	211	207	-0.21
4	118	116	3.04
6	147	148	-0.44
-8	91	84	2.93
-6	258	251	-0.05
-4	133	131	-1.77
-2	148	156	-1.98
H= 15, K= 2			
1	194	191	1.00
3	110	101	-0.41
5	37	42	0.26
-7	-26	47	-0.79
-5	134	129	-1.41
-3	115	115	2.97
-1	109	96	-1.49
H= 16, K= 2			
0	67	77	2.83
2	200	209	3.04
4	83	76	-0.13
-6	148	143	2.73
-4	219	217	0.07
-2	99	102	-2.22
H= 17, K= 2			
1	-24	23	-0.96
3	99	98	1.08
-5	-24	5	-1.90
-3	116	112	-2.46
-1	193	195	2.56
H= 18, K= 2			
0	-25	15	0.03
2	134	132	1.28
-6	121	132	0.38
-4	91	95	3.08
-2	233	239	0.03
H= 19, K= 2			
1	135	134	2.25
-5	95	93	-1.00
-3	-27	52	-3.06
-1	95	105	-2.42
H= 20, K= 2			
0	129	136	-0.61
-4	95	100	-0.47
-2	193	195	-2.47
H= 21, K= 2			
-3	117	108	-1.49

L	FO	FC	ALPHA
-1	38	44	-2.57
H= 0, K= 3			
1	132	120	3.03
3	525	519	-1.83
5	186	192	2.33
7	173	183	-1.88
9	71	66	1.38
H= 1, K= 3			
0	562	552	-2.78
2	208	206	-2.00
4	497	508	-2.99
6	157	152	-0.09
8	98	105	-2.52
-8	147	140	2.23
-6	92	88	0.39
-4	281	284	2.88
-2	568	575	-0.12
H= 2, K= 3			
1	234	223	1.32
3	311	302	1.62
5	140	133	-1.90
7	189	189	1.91
9	61	52	-2.56
-9	90	88	1.16
-7	187	190	-1.07
-5	348	347	1.37
-3	85	85	-1.28
-1	853	818	1.41
H= 3, K= 3			
0	725	727	-0.13
2	446	433	-2.87
4	103	95	-0.15
6	186	188	2.80
8	121	123	0.23
-8	-24	28	-0.56
-6	168	166	2.01
-4	416	408	0.11
-2	135	136	0.92
H= 4, K= 3			
1	306	308	0.66
3	208	206	-1.07
5	107	108	0.94
7	135	133	-1.02
-9	86	81	-1.69
-7	48	52	1.86
-5	480	472	-1.55
-3	297	285	1.48
-1	382	392	-1.34
H= 5, K= 3			
0	163	156	0.68
2	440	427	-0.21
4	190	192	3.11
6	166	172	0.54
8	92	94	2.04
-8	189	191	-2.89
-6	66	63	-1.75
-4	152	147	1.31
-2	766	771	0.16
H= 6, K= 3			
1	240	216	-1.82
3	38	49	1.27
5	180	175	-1.97
7	65	67	2.59
-9	41	35	1.70
-7	80	76	-2.03
-5	243	242	1.86

L	FO	FC	ALPHA
-3	520	509	-1.90
-1	527	513	1.85
H= 7, K= 3			
0	284	290	0.05
2	424	411	-2.63
4	204	208	-1.41
6	183	191	-2.81
8	53	46	-0.09
-8	37	45	-0.58
-6	441	453	-3.14
-4	218	206	-3.13
-2	167	195	2.27
H= 8, K= 3			
1	519	497	1.57
3	-21	18	-0.43
5	101	106	1.54
7	52	63	-2.56
-9	-26	31	-1.10
-7	82	87	0.39
-5	103	116	-1.18
-3	413	426	1.49
-1	344	331	-1.77
H= 9, K= 3			
0	103	108	1.43
2	198	212	-0.12
4	224	226	-2.66
6	56	56	-0.98
-8	38	41	3.07
-6	140	139	-0.39
-4	386	388	3.01
-2	170	184	1.18
H= 10, K= 3			
1	392	395	-1.36
3	217	206	0.90
5	122	126	-0.59
7	84	78	0.38
-7	79	70	-1.73
-5	131	134	-1.01
-3	372	387	-1.57
-1	248	239	1.23
H= 11, K= 3			
0	364	357	0.76
2	47	44	-0.13
4	180	175	0.03
6	68	70	3.07
-8	167	171	-0.28
-6	56	61	-2.40
-4	297	294	-0.19
-2	215	224	2.21
H= 12, K= 3			
1	220	214	1.88
3	218	220	-1.76
5	-26	52	1.68
-7	204	211	1.74
-5	102	106	2.45
-3	62	70	-2.69
-1	364	383	-2.05
H= 13, K= 3			
0	201	225	2.60
2	103	106	0.27
4	155	159	-1.88
6	81	84	-0.64
-8	143	139	-3.10
-6	102	101	-1.12
-4	230	220	-2.87
-2	201	191	0.02

L	FO	FC	ALPHA
H= 14, K= 3			
1	169	185	-2.21
3	216	215	1.74
5	62	63	-2.39
-7	144	145	-1.35
-5	246	255	1.44
-3	198	201	1.69
-1	134	132	1.86
H= 15, K= 3			
0	228	228	0.57
2	135	141	2.45
4	76	82	0.42
-6	197	196	-2.93
-4	93	98	-1.18
-2	173	172	2.76
H= 16, K= 3			
1	84	83	0.84
3	140	135	-1.37
-7	37	48	0.27
-5	294	293	-1.33
-3	109	106	0.74
-1	82	90	0.88
H= 17, K= 3			
0	149	153	2.20
2	184	188	0.48
4	65	57	2.29
-6	133	126	-0.59
-4	210	204	-2.73
-2	-25	65	-0.16
H= 18, K= 3			
1	-25	19	2.52
3	-26	38	2.16
-5	66	72	1.69
-3	268	258	-1.61
-1	-24	25	-3.06
H= 19, K= 3			
0	-25	12	-2.03
2	83	87	3.08
-4	135	148	-1.22
-2	242	233	-2.78
H= 20, K= 3			
1	62	49	2.37
-3	142	148	1.62
-1	125	129	-1.69
H= 21, K= 3			
-2	81	85	-0.66
H= 0, K= 4			
0	-20	30	-3.14
2	253	250	0.22
4	253	259	0.33
6	114	117	0.07
8	57	62	0.76
H= 1, K= 4			
1	250	224	-1.57
3	386	379	1.95
5	111	114	-2.33
7	285	287	1.63
9	-26	40	-0.42
-9	41	36	0.70
-7	47	56	-2.08
-5	532	525	1.40
-3	259	290	-0.99
-1	148	145	0.0
H= 2, K= 4			
0	218	240	-2.00
2	185	192	-2.49
4	105	112	-1.13
6	115	115	-0.23
8	67	70	-1.00
-8	104	101	3.00
-6	90	84	-2.70
-4	37	44	-0.68
-2	147	144	-1.88
H= 3, K= 4			
1	604	565	-1.33
3	423	409	-1.51
5	163	170	1.73
7	168	165	-1.27
-9	149	149	-1.89
-7	47	51	-3.01
-5	203	199	-2.12
-3	519	500	1.50
-1	844	853	-1.38
H= 4, K= 4			
0	329	304	2.81
2	220	234	2.96
4	147	155	2.53
6	90	91	3.11
8	-24	16	1.82
-8	38	40	1.43
-6	102	103	2.31
-4	158	155	2.26
-2	113	103	1.58
H= 5, K= 4			
1	447	415	-1.40
3	107	102	-2.78
5	197	186	-2.31
7	176	177	2.03
-9	65	71	1.60
-7	99	98	-1.86
-5	256	265	1.65
-3	38	43	2.75
-1	736	722	1.47
H= 6, K= 4			
0	140	141	-0.78
2	48	53	2.20
4	43	65	1.96
6	100	101	1.23
8	-25	25	2.40
-8	66	57	-0.71
-6	109	99	-0.25
-4	92	88	-0.32
-2	70	67	1.32
H= 7, K= 4			
1	485	470	1.21
3	177	176	-1.52
5	125	131	2.30
7	71	80	-2.27
-9	72	78	-1.38
-7	109	106	1.58
-5	79	69	-1.92
-3	362	369	1.55
-1	231	249	-0.90
H= 8, K= 4			
0	86	83	-2.23
2	234	240	-1.55
4	74	72	-1.29
6	39	36	-1.96
-8	45	57	-2.49
-6	60	73	-1.58
-4	115	112	-0.32
-2	143	150	-1.21
H= 9, K= 4			
1	553	569	-1.00
3	195	200	0.55
5	160	166	-1.31
7	58	48	0.95
-7	168	164	-1.85
-5	145	147	2.28
-3	227	229	-1.89
-1	121	124	0.78
H= 10, K= 4			
0	-22	21	-2.09
2	105	96	2.18
4	105	95	-2.40
6	-25	30	3.11
-8	61	55	2.50
-6	82	89	2.58
-4	51	56	1.42
-2	216	223	0.79
H= 11, K= 4			
1	204	200	1.56
3	224	229	-1.35
5	110	113	2.10
-7	103	105	1.66
-5	112	110	3.08
-3	439	441	2.01
-1	102	103	-2.38
H= 12, K= 4			
0	249	253	0.43
2	52	67	-0.32
4	113	119	1.04
6	-25	12	1.97
-8	93	100	0.23
-6	-23	18	-1.74
-4	60	72	2.47
-2	50	66	1.09
H= 13, K= 4			
1	113	119	-0.71
3	146	148	1.48
5	101	105	-1.55
-7	239	244	-1.34
-5	80	89	1.91
-3	113	135	2.92
-1	403	397	1.75
H= 14, K= 4			
0	126	124	-2.59
2	145	136	-0.42
4	93	97	-1.33
-6	73	79	-0.21
-4	92	82	-2.06
-2	132	142	-3.10
H= 15, K= 4			
1	232	224	1.08
3	212	218	-0.67
5	64	64	0.61
-7	64	71	0.83
-5	346	346	-1.51
-3	99	88	-2.67
-1	147	144	-1.84

```
  L    FO      FC    ALPHA

 H=   16.  K=    4

  0   158     161     2.76
  2   158     159    -3.04
  4   -25      26    -1.03
 -6    88      95    -3.10
 -4   102     107     0.47
 -2    45      43     2.60

 H=   17.  K=    4

  1    99     103    -2.19
  3   154     153     1.54
 -5   181     179     1.63
 -3   221     222    -2.11
 -1   156     155     2.81

 H=   18.  K=    4

  0    65      64     0.51
  2    77      69     1.72
 -4   -25      31    -2.96
 -2   164     165     0.37

 H=   19.  K=    4

  1    93     105     2.01
 -5    98      99    -1.19
 -3   223     217     1.86
 -1   109     125    -2.41

 H=   20.  K=    4

  0    97      96    -0.09
 -4    41      41    -0.62
 -2    68      61    -2.56

 H=    0.  K=    5

  1   337     323     2.24
  3   165     156     2.50
  5    83      78    -2.73
  7    39      32    -1.50

 H=    1.  K=    5

  0   700     690    -2.90
  2   236     230    -1.58
  4   478     479    -2.96
  6   222     217    -0.31
  8   100     103    -3.00
 -8   196     190     2.88
 -6   142     142     1.00
 -4   584     594     3.09
 -2   120     112    -0.21

 H=    2.  K=    5

  1   168     169    -1.11
  3   225     219     1.84
  5   103      92     1.29
  7   -23      17     1.07
 -9    49      53     0.64
 -7   -23      43     0.12
 -5   119     126    -0.54
 -3    94     102    -1.09
 -1   110     116    -0.52

 H=    3.  K=    5

  0   108     115     0.21
  2   532     521    -3.13
  4   130     118    -0.44
  6   280     277     2.94
  8    95      93     0.11
 -8   132     132     0.34
 -6   162     168     2.66
 -4   469     479     0.38
 -2   536     538     2.99
```

```
  L    FC      FC    ALPHA

 H=    4.  K=    5

  1    72      76     0.75
  3   133     136    -1.10
  5   -23      34     1.31
  7    59      66     0.15
 -9    45      35    -2.23
 -7    72      79     1.02
 -5    54      50    -0.65
 -3   326     322    -1.27
 -1   236     232    -1.30

 H=    5.  K=    5

  0   282     280    -3.14
  2   236     232    -0.28
  4   203     193     2.89
  6   236     226     0.11
  8    91     102     2.44
 -8   141     133    -2.44
 -6   253     248    -0.03
 -4   -20      11     2.37
 -2   907     929     0.09

 H=    6.  K=    5

  1   183     188    -2.60
  3   192     202     2.57
  5   103     100    -1.96
  7    52      49    -2.29
 -9    43      43     1.60
 -7    79      78     2.61
 -5   184     184     1.74
 -3    82      89    -3.01
 -1   335     321    -1.81

 H=    7.  K=    5

  0   629     612    -0.11
  2   461     459    -2.75
  4   176     185    -1.54
  6   186     184    -2.92
 -8   -24      10     1.64
 -6   348     345    -3.05
 -4   194     202     0.31
 -2   193     198     3.03

 H=    8.  K=    5

  1    84      60    -1.39
  3    94      98     2.36
  5   165     170     1.91
  7   -25      14     0.91
 -7    84      90     0.94
 -5    46      46     1.29
 -3   205     194     0.98
 -1   150     129     0.64

 H=    9.  K=    5

  0   173     174     2.26
  2   450     449     0.0
  4   237     228     3.14
  6   -24      20    -0.97
 -8   145     141    -2.89
 -6    38      50     0.80
 -4   353     348     2.93
 -2   444     454     0.45

 H=   10.  K=    5

  1   118     121     0.28
  3    59      52    -1.98
  5   -24       9     1.55
  7    69      78     1.34
 -7    52      46    -3.09
 -5    54      62     0.81
 -3   111     110    -0.98
 -1   173     175    -0.02
```

```
  L    FO      FC    ALPHA

 H=   11.  K=    5

  0   467     464     0.31
  2    63      81     2.28
  4   313     307     0.02
  6    75      87     2.39
 -8   208     208    -0.14
 -6   195     201    -2.53
 -4   134     131     0.04
 -2   261     259     2.70

 H=   12.  K=    5

  1    80      74    -1.20
  3    35      43    -2.08
  5   109     110    -2.36
 -7    49      49    -3.12
 -5   118     120     2.86
 -3    48      41    -2.92
 -1   147     153    -1.49

 H=   13.  K=    5

  0   342     340    -3.13
  2   187     180    -0.51
  4   172     172    -2.51
 -6   119     130    -0.55
 -4   333     340    -2.84
 -2    44      55    -0.16

 H=   14.  K=    5

  1    58      65    -0.55
  3   -24      20     1.49
  5   -25      27     1.64
 -7   -25       7     2.27
 -5    72      76     1.92
 -3    48      56     1.46
 -1    66      64     0.16

 H=   15.  K=    5

  0   199     198     0.54
  2   199     203     2.95
  4    76      70    -0.32
 -6   203     207    -2.85
 -4   134     143    -0.09
 -2   219     229     2.75

 H=   16.  K=    5

  1    73      77    -0.16
  3    40      44    -0.72
 -5    44      45     2.88
 -3    64      68     1.83
 -1   111     110     0.15

 H=   17.  K=    5

  0   169     168     2.06
  2   255     254     0.29
 -6   228     225    -0.16
 -4   204     203    -2.76
 -2   163     166     0.21

 H=   18.  K=    5

  1    58      66    -0.16
 -5    76      71     2.96
 -3    96     101    -3.06
 -1    54      62     2.32

 H=   19.  K=    5

  0    47      38    -0.51
 -4   176     173    -0.63
 -2   279     279    -2.86
```

```
   L     FO      FC    ALPHA

H=   20,  K=     5

  -3     40      54     2.37
  -1    -27      27     2.65

H=    0,  K=     6

   0     57      55     0.0
   2    256     257     2.76
   4    113     121     2.57
   6    127     131     0.37
   8    -24       5    -2.55

H=    1,  K=     6

   1    965     649    -1.54
   3    460     446     1.55
   5    121     117    -1.51
   7    230     234     1.49
  -7    137     139    -1.35
  -5    352     354     1.35
  -3    321     315    -1.10
  -1    497     490     1.18

H=    2,  K=     6

   0    501     488    -2.71
   2    188     189    -0.71
   4     54      54     0.55
   6     43      38    -2.46
   8     51      54    -0.34
  -8    -25       3    -0.13
  -6     37      37    -1.31
  -4    290     294    -0.47
  -2    259     259    -2.35

H=    3,  K=     6

   1    205     198     0.94
   3    748     737    -1.63
   5    175     169     1.13
   7    171     174    -1.18
  -7    126     126     2.02
  -5    272     281    -1.87
  -3    354     344     1.48
  -1    654     642    -1.43

H=    4,  K=     6

   0    187     185    -3.05
   2    368     352     2.99
   4    106     104     0.74
   6     99     101     1.19
   8     52      48    -3.07
  -8     54      57     1.24
  -6    106     113     0.53
  -4    101     105     0.71
  -2    360     342     0.10

H=    5,  K=     6

   1    309     290    -1.93
   3    360     375     1.87
   5    341     331    -2.16
   7    125     134     1.88
  -7    146     150    -1.90
  -5    371     364     1.70
  -3    101     112    -2.46
  -1    684     687     1.55

H=    6,  K=     6

   0    227     231    -0.48
   2     86      95    -1.80
   4    132     132     2.72
   6     55      57     0.48
  -8     51      54     2.57
  -6     63      65     0.81
  -4    146     153     0.12

   L     FO      FC    ALPHA

  -2     87      70    -2.82

H=    7,  K=     6

   1    567     556     1.33
   3    138     126    -1.73
   5    280     289     1.64
   7    107     105    -2.41
  -7    178     180     1.31
  -5    239     241    -1.58
  -3    405     399     1.33
  -1    181     178    -0.94

H=    8,  K=     6

   0    291     290    -2.56
   2    182     185    -0.89
   4     96      93    -0.70
   6    -24      33     2.11
  -8    -26      45    -3.06
  -6     52      49     2.64
  -4     90      88     0.28
  -2    103     102    -0.57

H=    9,  K=     6

   1    473     470    -1.27
   3    193     196     0.82
   5    197     197    -1.28
   7    110     109     0.95
  -7    283     285    -1.64
  -5    145     147     1.76
  -3    427     441    -1.69
  -1    154     161     0.58

H=   10,  K=     6

   0     73      74    -3.05
   2    298     302    -3.04
   4    -23      14     2.50
   6    -25      10     1.70
  -8    -26      27    -2.97
  -6     75      76     1.26
  -4    155     159     1.14
  -2    106     114     1.19

H=   11,  K=     6

   1    156     152     1.65
   3    288     295    -1.79
   5    100      99     2.07
  -7    202     208     1.65
  -5    244     249    -1.97
  -3    392     381     1.87
  -1    238     244    -2.08

H=   12,  K=     6

   0     67      70    -1.10
   2     80      82    -1.92
   4    149     149     3.09
   6    -25      22     0.95
  -6     52      42    -2.83
  -4    161     165     0.55
  -2    183     193     0.46

H=   13,  K=     6

   1     68      69    -1.16
   3    181     177     1.36
   5    117     124    -1.65
  -7    128     128    -1.35
  -5    255     264     1.44
  -3    197     221    -1.83
  -1    407     402     1.53

H=   14,  K=     6

   0    197     196    -0.15
   2    138     140    -1.19

   L     FO      FC    ALPHA

   4     63      60    -1.32
  -6     96      92    -2.77
  -4     43      36     2.50
  -2    194     192     0.40

H=   15,  K=     6

   1    221     222     1.11
   3    139     142    -0.82
  -5    244     245    -1.64
  -3    159     162     1.41
  -1    280     289    -1.61

H=   16,  K=     6

   0     99      97     0.86
   2     94      91    -0.18
  -6     61      52    -2.91
  -4    110     106     2.40
  -2    134     141     2.09

H=   17,  K=     6

   1    194     198    -2.07
   3    109     120     1.77
  -5    121     120     1.84
  -3    206     215    -2.12
  -1    201     201     1.84

H=   18,  K=     6

   0     60      60     2.25
   2    -27      33    -0.04
  -4     56      50     2.46
  -2     74      84     1.88

H=   19,  K=     6

   1    176     183     1.49
  -3    118     125     1.60
  -1    113     121    -1.97

H=    0,  K=     7

   1    245     260     2.41
   3    300     310     1.90
   5    174     176    -1.65
   7    -24      31    -0.06

H=    1,  K=     7

   0    552     549    -2.95
   2    213     207    -0.45
   4    185     195    -2.56
   6    101      98    -1.08
   8    112     116    -2.80
  -8    152     147    -3.06
  -6    101     101     0.59
  -4    202     195     3.14
  -2     74      63    -1.85

H=    2,  K=     7

   1     84      95     2.91
   3    199     188     1.47
   5    195     196     1.34
   7     90      95    -1.21
  -7    110     104     1.30
  -5    160     163    -0.89
  -3    153     147     1.10
  -1    280     294    -1.60

H=    3,  K=     7

   0    249     247     0.56
   2    394     380     2.88
   4    179     173     0.76
   6    109     114     2.78
   8    -25      32     0.41
  -8    147     144     0.32
```

```
   L     FO      FC    ALPHA

  -6    117     117     2.90
  -4    303     308     0.57
  -2    142     148     2.07

H=    4,  K=      7

   1     73      73    -3.06
   3    193     203     2.17
   5    113     113     1.06
   7    106     109     1.24
  -7    -23      17    -1.15
  -5    157     157     1.06
  -3    342     345    -1.20
  -1    191     187     1.27

H=    5,  K=      7

   0     67      64    -0.92
   2    397     398     0.09
   4    120     119     2.90
   6    174     179     0.40
  -8    137     136    -2.71
  -6    179     171    -0.23
  -4    168     166    -2.57
  -2    376     365    -0.05

H=    6,  K=      7

   1    152     146     2.51
   3    148     148    -3.00
   5    104     101     2.74
   7     54      49    -0.55
  -7    159     156     1.92
  -5     51      47    -2.56
  -3     57      62     0.22
  -1    556     565    -1.57

H=    7,  K=      7

   0    193     197    -0.87
   2    257     256    -2.51
   4    152     156    -0.40
   6    155     155    -2.62
  -8     68      72     0.12
  -6    289     290    -3.04
  -4    -22       5    -2.94
  -2    432     429    -2.89

H=    8,  K=      7

   1    441     455    -1.55
   3    106     106     2.14
   5    -24      19     2.34
   7    -26      39     1.80
  -7    -24      28    -2.41
  -5    216     217     1.46
  -3    136     145    -0.82
  -1    225     233    -0.35

H=    9,  K=      7

   0    337     328     2.91
   2    151     151     0.09
   4    198     193     3.05
   6     66      68     0.82
  -8     47      44     2.71
  -6    262     259     0.31
  -4    235     230     2.82
  -2    138     137     1.10

H=   10,  K=      7

   1    112     105     0.14
   3    241     248    -1.98
   5     90      93     2.16
  -7    -25      33     1.21
  -5     34      44     2.21
  -3    286     284     1.25
  -1    139     146    -0.41
```

```
   L     FO      FC    ALPHA

H=   11,  K=      7

   0    213     206     0.07
   2    121     121     2.64
   4    219     216     0.03
   6     63      58     2.66
  -6     81      74    -2.35
  -4    391     395     0.07
  -2     72      72    -3.00

H=   12,  K=      7

   1     67      59    -0.95
   3    -23      12     2.69
   5    165     164    -2.14
  -7     83      87    -2.94
  -5     71      78     2.59
  -3     44      39    -2.60
  -1    194     202     1.10

H=   13,  K=      7

   0    167     173    -2.55
   2    132     134    -0.84
   4    123     134    -2.92
  -6     49      47    -0.80
  -4    254     246    -2.91
  -2    237     232    -0.05

H=   14,  K=      7

   1    166     166     0.89
   3    -25      18     0.75
  -5     70      70     3.13
  -3     43      18     0.98
  -1    120     121    -0.55

H=   15,  K=      7

   0    168     170     0.49
   2    106     112     2.91
   4    -26      28    -0.02
  -6     40      50     2.47
  -4    113     107     0.61
  -2    270     271     2.94

H=   16,  K=      7

   1    111     116    -0.83
   3     48      51     1.32
  -5     91      95     2.31
  -3     49      43     2.70
  -1     49      53     0.14

H=   17,  K=      7

   0    138     143     3.02
   2    173     107     0.29
  -4    -25       9    -2.17
  -2    165     169     0.16

H=   18,  K=      7

   1     41      44    -0.52
  -3     99     103     2.59
  -1    -26      12    -0.22

H=   19,  K=      7

   0    118     117    -0.44
  -2    113     110    -2.54

H=    0,  K=      8

   0    451     430    -3.14
   2     70      56     1.12
   4    110     109     2.32
   6    105     106    -0.22
   8     68      68    -1.62
```

```
   L     FO      FC    ALPHA

H=    1,  K=      8

   1    122     128     0.10
   3    292     295     1.35
   5     37      45    -0.39
   7    182     182     1.34
  -7    212     218    -0.97
  -5    144     140     1.23
  -3    149     157    -0.69
  -1    438     441     1.22

H=    2,  K=      8

   0    124     117    -0.63
   2    233     225    -3.11
   4    159     155     0.35
   6     59      54     1.63
  -8    -27      33    -1.91
  -6     63      66     0.36
  -4    188     183    -0.22
  -2    185     179    -2.23

H=    3,  K=      8

   1    218     225     1.55
   3    257     251    -1.13
   5     62      70     0.07
   7    117     115    -1.17
  -7     84      84     2.63
  -5    422     419    -1.52
  -3     76      61     2.77
  -1    283     265    -1.62

H=    4,  K=      8

   0    270     252    -2.95
   2    112     112     0.60
   4    146     148     2.58
   6    101      99     0.57
  -8     96      93     2.83
  -6    -23       6     0.61
  -4    135     140     0.16
  -2    154     137     0.02

H=    5,  K=      8

   1    229     217    -2.48
   3    252     251     2.14
   5    141     140    -1.68
   7     36      43    -2.92
  -7     59      65    -1.88
  -5    204     200     2.03
  -3    422     419    -1.70
  -1    259     261     2.14

H=    6,  K=      8

   0    113     106    -1.57
   2    316     312    -2.84
   4     69      68     0.27
   6     74      71     3.09
  -8    110     105     0.41
  -6    124     111     2.74
  -4     49      46    -3.10
  -2     88      98    -1.21

H=    7,  K=      8

   1    301     292     1.39
   3     47      53    -0.96
   5    207     207     1.54
   7     51      34    -0.20
  -7    199     197     1.28
  -5    138     147    -0.96
  -3    253     240     1.11
  -1    365     365    -1.39

H=    8,  K=      8

   0    145     152    -1.44
   L    FO      FC    ALPHA

   2   116     112    -0.60
   4   143     139    -3.10
   6    88      92     0.32
  -6   230     239     0.25
  -4    33      36     0.76
  -2    33      36    -2.15

H=    9, K=      8

   1   385     385    -1.71
   3   115     114     0.97
   5   151     147    -0.98
  -7   137     126    -1.73
  -5   155     161     1.63
  -3   209     220    -1.48
  -1   161     153     1.10

H=   10, K=      8

   0    69      80    -3.08
   2   101     103    -2.40
   4    84      68     0.51
   6    88      93     2.79
  -6   117     122     2.71
  -4   361     368     0.39
  -2    76      74     0.57

H=   11, K=      8

   1   229     221     1.98
   3   298     286    -2.31
   5    66      70     2.08
  -7    87      93     1.85
  -5   134     134    -1.94
  -3   232     241     1.83
  -1   131     134    -2.59

H=   12, K=      8

   0    88      91    -1.36
   2    87      94    -2.53
   4   107     103    -2.55
  -6    48      33     2.44
  -4   175     177     2.75
  -2   308     307     0.22

H=   13, K=      8

   1   -25      31     2.63
   3   215     210     1.51
  -5   107     111     0.94
  -3   213     205    -0.99
  -1   219     223     1.24

H=   14, K=      8

   0   263     255    -0.02
   2    88      91    -1.21
   4   -26      21     2.69
  -6   117     119    -2.93
  -4    84      83     0.92
  -2   128     133     2.66

H=   15, K=      8

   1    73      67     0.37
   3    86      84    -1.44
  -5   102      99    -1.49
  -3    65      68     0.32
  -1   281     275    -1.12

H=   16, K=      8

   0   112     112     2.87
   2   137     133    -0.21
  -4   146     137     2.70
  -2   127     132     0.93

H=   17, K=      8
```

```
   L    FO      FC    ALPHA

   1   163     151    -1.64
  -3    61      72    -1.99
  -1   108     102     1.87

H=   18, K=      8

   0    99      98     0.28
  -2   115     123     2.64

H=    0, K=      9

   1   349     343    -1.82
   3   238     231     1.63
   5   122     123    -1.37
   7    79      84     2.15

H=    1, K=      9

   0   223     222    -2.94
   2   121     128    -0.40
   4   123     125    -2.70
   6   130     131    -0.57
  -6    41      40    -1.28
  -4   304     304    -3.10
  -2    39      40    -2.56

H=    2, K=      9

   1   329     322     1.76
   3   278     274    -1.54
   5    97      97     0.94
   7   147     145    -1.34
  -7   114     113    -0.47
  -5   159     150    -1.71
  -3    46      51     0.72
  -1   423     400    -1.68

H=    3, K=      9

   0   186     181     1.10
   2   207     212     2.11
   4   122     128     1.10
   6   157     156     2.77
  -6    61      58     1.19
  -4   134     139     0.49
  -2   310     303     2.67

H=    4, K=      9

   1   266     255    -1.93
   3   370     365     1.76
   5    94      96    -1.67
   7    80      70     1.26
  -7    42      45     2.51
  -5   153     153    -0.20
  -3   125     124    -1.27
  -1   162     154     1.48

H=    5, K=      9

   0   112     106    -2.66
   2   243     238     0.06
   4    63      57     0.85
   6   109     113     0.08
  -6   148     154    -0.94
  -4    98      98    -1.92
  -2   197     191    -0.56

H=    6, K=      9

   1   154     163     1.86
   3   198     199    -1.88
   5   206     200     1.66
  -7   236     237     1.63
  -5    70      61     2.11
  -3   156     161    -0.80
  -1   176     174    -1.43

H=    7, K=      9
```

```
   L    FO      FC    ALPHA

   0   111     106    -1.15
   2   117     117    -2.64
   4   112     114    -0.40
   6    51      55    -1.93
  -6    39      52    -3.04
  -4   124     126    -1.84
  -2   284     277    -2.09

H=    8, K=      9

   1   152     156    -1.38
   3   141     150     1.71
   5   129     125    -1.52
  -7   181     184    -1.77
  -5   255     262     1.55
  -3    53      55     0.64
  -1   157     167    -1.22

H=    9, K=      9

   0   252     242     2.95
   2   119     122     1.37
   4   132     132     2.44
  -6   182     184     0.48
  -4    97      98     1.78
  -2    48      59     2.83

H=   10, K=      9

   1   102      96    -2.72
   3    71      64    -2.04
   5   146     147     1.92
  -7   101     114     1.66
  -5   207     211    -1.68
  -3   276     278     1.43
  -1    87      93     0.78

H=   11, K=      9

   0    81      82    -0.99
   2    53      53    -3.03
   4   139     131     0.57
  -6   -25      13     2.37
  -4   200     206    -0.15
  -2    69      63    -1.65

H=   12, K=      9

   1    91      83    -0.46
   3   101      96    -2.90
  -5   152     159     1.63
  -3   283     290    -1.48
  -1   127     133     1.07

H=   13, K=      9

   0   160     169    -2.21
   2    67      64    -1.63
   4    74      75    -2.42
  -6    40      55     0.09
  -4    90      80    -3.08
  -2   136     130    -1.00

H=   14, K=      9

   1    73      58     0.50
   3    89      97    -0.71
  -5    83     100    -2.17
  -3   202     209     1.40
  -1   276     278    -1.29

H=   15, K=      9

   0   -25      24    -0.81
   2   118     119    -3.14
  -4   131     137     0.74
  -2   100     105     2.62
```

```
   L    FO      FC   ALPHA

H=  16, K=    9

   1   155     157   -1.54
  -3    56      57   -2.75
  -1   243     252    1.47

H=  17, K=    9

   0   -26      24   -1.67
  -2   154     158   -0.03

H=   0, K=   10

   0   394     393    3.14
   2    39      36    0.96
   4   214     218    3.09
   6   217     212   -0.27

H=   1, K=   10

   1   322     318    1.16
   3   178     184    0.44
   5   151     152   -0.91
   7   -25      18    3.05
  -7   -26      31    0.99
  -5   118     128   -0.74
  -3   188     185   -1.32
  -1    92      89    0.87

H=   2, K=   10

   0   160     156    0.07
   2   250     250    2.97
   4   100     102    0.58
   6   129     135    2.85
  -6    80      63    2.58
  -4   385     389    0.05
  -2   147     149   -2.95

H=   3, K=   10

   1   -23      24   -2.34
   3   101     100    0.75
   5   110     109   -0.05
  -7    96      99   -1.01
  -5    63      58    2.78
  -3   104     102   -2.18
  -1   136     134   -2.23

H=   4, K=   10

   0   161     153   -2.98
   2   175     178    0.19
   4   133     130    3.08
   6    86      90    0.15
  -6    61      62   -0.12
  -4   113     111   -3.07
  -2   428     438   -0.13

H=   5, K=   10

   1   205     209    2.81
   3    86      86   -2.97
   5   -24      32   -3.06
  -7   102      97    1.80
  -5    95      93   -1.49
  -3   157     158    2.26
  -1   247     258    2.70

H=   6, K=   10

   0   289     296   -0.30
   2   233     228   -3.12
   4    97      95    0.14
   6   100      99   -2.73
  -6   200     205    3.13
  -4   -24      34    0.47
  -2   234     246   -2.99

   L    FO      FC   ALPHA

H=   7, K=   10

   1   209     209    1.90
   3   135     136    1.46
   5    75      73    0.80
  -7    54      51   -0.40
  -5   103     114    0.08
  -3   206     208   -1.02
  -1   180     185    1.06

H=   8, K=   10

   0   171     178   -3.09
   2   227     230   -0.08
   4   154     153    2.70
  -6   206     205    0.25
  -4   159     162    2.99
  -2   149     143    0.10

H=   9, K=   10

   1    52      52    0.62
   3    52      51    2.38
   5    41      46    0.04
  -5   125     121   -1.42
  -3   141     152   -1.02
  -1   252     243   -1.79

H=  10, K=   10

   0   169     167   -0.14
   2   142     149   -3.03
   4   143     140   -0.13
  -6   137     129   -3.11
  -4   228     230    0.15
  -2   138     137   -3.06

H=  11, K=   10

   1   256     256   -2.59
   3   -26      17    3.07
  -5   -25      13   -0.52
  -3    92      94   -1.82
  -1   108      98   -1.87

H=  12, K=   10

   0   168     158   -2.85
   2   100     104   -0.48
   4   142     140   -2.88
  -4   213     216    3.13
  -2   169     171   -0.03

H=  13, K=   10

   1    56      42    0.43
   3   106     113    2.91
  -5   127     120    1.10
  -3   131     135    0.10
  -1    62      62    0.28

H=  14, K=   10

   0   180     182    0.08
   2    94      91    3.01
  -4    94      93    0.39
  -2   170     167    2.97

H=  15, K=   10

   1   -26      13   -2.08
  -3    77      78    0.34
  -1    96      91   -0.75

H=  16, K=   10

   0   106     114    3.10
  -2   109     106    0.22

H=   0, K=   11

   L    FO      FC   ALPHA

   1   122      99   -1.06
   3   120     118    1.05
   5   256     251   -1.54

H=   1, K=   11

   0    96     102    0.02
   2    54      49   -2.80
   4   107     104   -2.34
   6   105     101   -1.07
  -6    74      74   -2.43
  -4   234     222   -2.85
  -2    37      36   -1.98

H=   2, K=   11

   1    65      56    2.28
   3   140     123   -1.35
   5    83      80    1.37
  -5   260     257   -1.61
  -3   360     352    1.70
  -1   100      88   -1.75

H=   3, K=   11

   0   158     155    1.54
   2   224     235    0.73
   4    83      89    1.70
   6   110     110    2.96
  -6   105      99    0.58
  -4    51      54    2.55
  -2   311     301    2.79

H=   4, K=   11

   1   -24      29    3.01
   3   137     142    2.09
   5    49      39   -1.92
  -5   199     205    1.66
  -3   278     269   -1.59
  -1   463     452    1.66

H=   5, K=   11

   0   229     225    3.10
   2    83      88    0.39
   4   225     225    0.06
  -6   104     102   -0.59
  -4   108     105   -0.86
  -2   115     120   -2.18

H=   6, K=   11

   1   298     284    1.36
   3    80      86   -0.70
   5    88      92    1.65
  -5   225     226   -1.29
  -3   211     216    1.40
  -1   381     376   -1.51

H=   7, K=   11

   0   121     125   -2.57
   2   184     183    2.93
   4   -24      18   -0.69
  -6   -25      19   -0.93
  -4    96     100   -1.07
  -2   106     111   -1.72

H=   8, K=   11

   1   404     399   -1.66
   3   128     120    0.97
   5   114     122   -1.11
  -5   102     103    1.87
  -3   282     283   -1.58
  -1   192     195    1.64
```

L	FO	FC	ALPHA
H=	9, K=	11	
0	37	39	2.42
2	135	133	2.29
4	179	182	2.39
-6	83	82	1.01
-4	41	54	1.06
-2	-24	23	-0.41
H=	10, K=	11	
1	260	256	1.75
3	233	226	-1.93
-5	58	60	-1.55
-3	226	225	1.67
-1	193	193	-1.95
H=	11, K=	11	
0	89	100	-1.04
2	71	70	-0.22
-4	80	79	-0.60
-2	92	94	-1.27
H=	12, K=	11	
1	141	139	-1.75
3	202	208	1.40
-5	80	75	1.14
-3	92	93	-1.03
-1	225	223	1.43
H=	13, K=	11	
0	115	119	-1.96
2	65	57	-1.87
-4	-26	34	-0.14
-2	103	102	-1.49
H=	14, K=	11	
1	120	123	1.48
-3	47	36	1.35
-1	129	130	-1.54
H=	15, K=	11	
0	-26	40	-2.39
-2	43	37	1.10
H=	0, K=	12	
0	123	120	3.14
2	139	141	-0.31
4	296	295	-2.99
6	84	83	-0.31
H=	1, K=	12	
1	381	384	1.29
3	74	82	0.26
5	55	47	0.60
-5	110	104	-1.38
-3	45	50	-0.85
-1	50	44	-0.14
H=	2, K=	12	
0	245	253	0.41
2	92	94	2.23
4	153	156	0.17
-6	122	124	2.84
-4	212	212	0.19
-2	225	229	2.82
H=	3, K=	12	
1	100	103	-1.77
3	218	213	1.13
5	60	50	-1.08
-5	-25	12	2.75
-3	150	150	-2.01
-1	110	107	-2.14
H=	4, K=	12	
0	136	141	-2.92
2	215	213	-0.06
4	40	42	-2.44
-6	108	115	-0.42
-4	213	212	-3.01
-2	291	286	-0.21
H=	5, K=	12	
1	129	131	-2.55
3	155	156	-2.07
5	67	79	1.16
-5	41	46	-2.17
-3	120	114	2.40
-1	132	136	-2.79
H=	6, K=	12	
0	228	225	-0.05
2	169	166	-3.06
4	87	75	-0.47
-4	72	77	-0.10
-2	295	298	3.09
H=	7, K=	12	
1	88	85	1.24
3	-25	32	0.27
-5	98	103	-0.38
-3	91	86	-0.78
-1	157	161	1.55
H=	8, K=	12	
0	237	233	2.71
2	219	214	0.32
4	102	107	2.78
-4	144	153	2.89
-2	164	169	0.30
H=	9, K=	12	
1	142	138	1.91
3	77	67	1.02
-5	56	52	-0.57
-3	71	71	-1.22
-1	86	92	-1.84
H=	10, K=	12	
0	190	192	0.0
2	125	130	2.91
-4	138	135	-0.56
-2	162	160	-2.90
H=	11, K=	12	
1	110	111	-2.47
-3	55	51	-1.58
-1	87	88	-2.69
H=	12, K=	12	
0	186	189	-3.06
2	97	96	0.04
-2	94	96	-0.67
H=	13, K=	12	
1	-27	47	2.31
-3	98	99	0.18
-1	61	62	-0.85
H=	0, K=	13	
1	196	203	-1.02
3	211	214	1.06
5	49	50	-1.06
H=	1, K=	13	
0	123	123	0.18
2	96	102	3.00
4	92	83	-0.42
-4	81	75	-0.85
-2	97	95	-3.03
H=	2, K=	13	
1	50	46	1.04
3	262	264	-1.62
5	75	75	1.21
-5	106	109	-2.18
-3	115	118	2.12
-1	249	254	-1.56
H=	3, K=	13	
0	113	113	2.10
2	140	151	0.47
4	102	107	2.57
-4	132	138	3.10
-2	68	65	0.50
H=	4, K=	13	
1	175	175	-1.62
3	73	72	1.47
-5	150	155	1.99
-3	57	53	3.02
-1	229	233	1.77
H=	5, K=	13	
0	44	41	-0.21
2	44	25	1.58
4	150	154	-0.21
-4	160	161	-0.43
-2	188	195	-2.82
H=	6, K=	13	
1	224	222	1.17
3	145	137	-0.91
-3	164	167	1.57
-1	41	43	-0.14
H=	7, K=	13	
0	202	206	-3.00
2	-24	11	2.05
-4	80	82	-2.84
-2	139	148	-0.53
H=	8, K=	13	
1	97	106	-1.75
3	82	85	1.16
-3	122	121	-2.00
-1	156	162	2.10
H=	9, K=	13	
0	99	94	0.13
2	170	168	2.82
-4	73	66	0.31
-2	115	108	2.89
H=	10, K=	13	
1	167	168	2.00
-3	150	152	2.12
-1	90	82	-2.78

```
   L     FO        FC   ALPHA

H=   11,  K=   13

   0     76        76   -2.90
  -2    118       119   -0.46

H=    0,  K=   14

   0    106       102    3.14
   2    160       160   -0.47
   4    124       131   -2.75

H=    1,  K=   14

   1     76        81    1.06
   3     57        67   -0.85
  -3     41        40    0.40
  -1     58        59   -1.01

H=    2,  K=   14

   0    280       277    0.42
   2     77        83    2.54
  -4     59        63    1.22
  -2    128       123    2.08

H=    3,  K=   14

   1     50        50   -0.93
   3     56        69    1.26
  -3     63        64   -1.69
```

```
   L     FO        FC   ALPHA

  -1    -25        27    2.08

H=    4,  K=   14

   0     45        51   -2.71
   2    243       244   -0.18
  -4    145       148   -2.60
  -2     51        46   -0.77

H=    5,  K=   14

   1     49        64    2.40
   3    -25        25   -1.43
  -3     76        85    1.97
  -1     59        63   -2.01

H=    6,  K=   14

   0    -25        38    1.00
   2    109       113   -3.06
  -2    176       176    3.00

H=    7,  K=   14

   1     52        61   -0.83
  -3     50        61   -1.37
  -1     67        70    1.66

H=    8,  K=   14

   0    163       162    2.14
```

```
   L     FO        FC   ALPHA

  -2     73        77    0.96

H=    9,  K=   14

  -1     85        94   -1.70

H=    0,  K=   15

   1    148       147   -0.76

H=    1,  K=   15

   0    176       176   -0.07
   2    186       185   -3.07
  -2     84        88    3.10

H=    2,  K=   15

   1     59        53    1.60
  -1    -25        24   -2.09

H=    3,  K=   15

   0    116       114    3.02
   2    134       138   -0.05
  -2    115       122   -0.02

H=    4,  K=   15

   1    -26         7   -1.89
  -1     87        95    1.94
```

```
   L     FO       FC    ALPHA

H=     0,  K=     0

   2    184      141     2.72
   4    241      259     0.16
   6    239      240     2.72
   8    226      230     0.44

H=     2,  K=     0

   0    955     1107     3.11
   2   1986     2433    -0.18
   4    476      493    -2.92
   6    122      122    -1.32
   8    162      161    -2.97
  -8    220      215    -3.11
  -6     49       72    -0.24
  -4    775      778     3.10
  -2    180      163     3.07

H=     4,  K=     0

   0    233      244     1.60
   2   1181     1273     3.00
   4    854      873    -0.41
   6    323      327     3.10
   8    -27       17    -1.72
  -8    205      202     0.02
  -6    392      384     2.97
  -4    113      108     1.78
  -2    947      950     2.82

H=     6,  K=     0

   0    337      373     1.59
   2    619      595     0.35
   4    559      571     2.86
   6    437      441    -0.31
   8    134      140     2.15
  -8     88       90    -2.65
  -6    451      443    -0.34
  -4    363      371    -2.93
  -2    431      451     0.11

H=     8,  K=     0

   0    324      326     0.08
   2    146      142     3.06
   4    282      280    -0.51
   6    320      327    -2.99
   8    214      221    -0.82
  -8    259      254    -0.04
  -6    355      352    -3.05
  -4    271      269    -0.90
  -2    670      666    -3.00

H=    10,  K=     0

   0    476      463     2.68
   2    320      341     0.53
   4    137      127    -3.01
   6    119      122    -0.51
  -8    208      207     3.05
  -6    406      411     0.0
  -4    534      525    -3.12
  -2    151      156    -0.65

H=    12,  K=     0

   0    356      364     0.25
   2    293      301     1.85
   4    322      345     0.54
   6    -27       38     1.77
  -8    285      283     0.11
  -6    228      229    -3.12
  -4    596      612    -0.27
  -2    311      309    -2.99

H=    14,  K=     0

   L     FO       FC    ALPHA

   0    369      366    -2.93
   2    120      127    -0.26
   4    141      133    -3.14
   6    135      131    -0.15
  -8    142      132     2.98
  -6    234      241    -0.07
  -4    553      552    -3.00
  -2    425      425    -0.80

H=    16,  K=     0

   0    203      204    -0.69
   2    257      254     2.39
   4    -27       43     0.05
  -6    140      133     2.58
  -4    274      279    -0.25
  -2    554      547    -3.07

H=    18,  K=     0

   0    277      278     2.88
   2    176      169     0.14
  -6    181      183     0.33
  -4     42       29     1.80
  -2    412      405    -0.27

H=    20,  K=     0

   0    281      279    -0.59
  -4     79       83    -0.15
  -2    152      143    -2.47

H=     0,  K=     1

   1    821      903     1.57
   3    190      217    -1.74
   5    134      124     3.02
   7    229      231    -2.04
   9     93       92     1.58

H=     1.  K=     1

   0    196      176    -2.53
   2    484      488     2.94
   4     63       61    -1.91
   6     46       50     0.35
   8     49       41     2.95
  -8     80       87     2.99
  -6     56       65     1.48
  -4    137      139     2.56
  -2    165      205    -3.01

H=     2,  K=     1

   1    894      961    -1.45
   3    664      671     1.40
   5     95       85     2.23
   7    228      225     2.08
   9     86       87    -2.49
  -9    117      117     1.10
  -7    195      200    -1.15
  -5    428      426     1.57
  -3    428      423     1.35
  -1    521      512     1.34

H=     3,  K=     1

   0     78      130    -2.70
   2    458      449    -2.42
   4    305      301     2.72
   6     36       16    -1.21
   8     52       54     0.37
  -8     48       43    -0.22
  -6    115      117     3.04
  -4    142      137     0.37
  -2     94       96     0.73

H=     4,  K=     1

   1    324      322    -0.80

   L     FO       FC    ALPHA

   3   1073     1132    -1.36
   5    224      234     0.63
   7    103      103    -0.78
  -9    179      178    -1.78
  -7     76       79     3.05
  -5    487      499    -1.68
  -3    322      327     1.92
  -1     94      113    -0.31

H=     5,  K=     1

   0    284      260     0.09
   2    127      127    -0.04
   4    230      230    -2.16
   6    161      154     2.23
   8    -26        7    -0.15
  -8     97       98    -2.99
  -6     96       95    -0.53
  -4    -21        9     1.10
  -2    507      494     0.05

H=     6,  K=     1

   1     39       46     1.63
   3     96      102     1.39
   5    514      513    -1.69
   7     75       80     1.65
  -9    113      109     1.49
  -7    224      219    -1.77
  -5    244      250     2.29
  -3    269      286    -2.23
  -1    708      735     1.95

H=     7.  K=     1

   0    432      400    -0.12
   2     64       78    -1.47
   4     82       93    -0.08
   6    137      139    -2.01
   8     80       72     2.25
  -8     82       68    -0.81
  -6    219      219     3.07
  -4     39       33    -0.99
  -2    106      107     1.16

H=     8,  K=     1

   1    640      668     1.70
   3    113      106     0.82
   5    252      255     1.74
   7    188      189    -2.19
  -9    130      125    -0.69
  -7    190      182     1.01
  -5    238      236    -1.26
  -3    543      545     1.75
  -1    158      150     2.56

H=     9,  K=     1

   0    156      158     1.29
   2    235      230    -0.29
   4     36       44    -2.31
   6     89       87     0.53
  -8     81       83     0.95
  -6     76       74    -0.81
  -4    262      258     3.00
  -2     55       53     1.25

H=    10,  K=     1

   1    367      349    -1.31
   3    232      230     0.67
   5    227      219    -0.60
   7    120      119     1.03
  -9    112      111     1.87
  -7    329      320    -1.37
  -5    -24       47    -0.75
  -3    441      437    -1.53
  -1    280      274     1.80
```

L	FO	FC	ALPHA
H= 11, K= 1			
0	74	81	1.54
2	73	85	1.97
4	105	108	-0.52
6	-26	32	3.09
-8	92	89	-2.62
-6	46	41	1.31
-4	59	61	-0.43
-2	195	193	2.63
H= 12, K= 1			
1	309	309	2.03
3	242	241	-1.60
5	68	54	1.44
-7	197	196	1.63
-5	361	356	-1.48
-3	221	209	2.25
-1	263	269	-2.38
H= 13, K= 1			
0	145	139	2.66
2	45	38	-2.43
4	66	69	-2.88
6	62	66	-1.28
-8	-28	24	0.23
-6	139	134	-2.75
-4	70	74	-2.81
-2	-24	37	1.38
H= 14, K= 1			
1	-25	136	-3.14
3	292	284	1.71
5	96	86	-1.86
-7	148	138	-0.74
-5	272	277	1.21
-3	261	254	-1.47
-1	377	380	2.06
H= 15, K= 1			
0	107	104	1.16
2	-25	54	2.16
4	60	28	-0.59
-6	74	70	-0.32
-4	62	50	-2.37
-2	36	42	-1.82
H= 16, K= 1			
1	133	131	1.71
3	104	108	-0.87
5	159	151	0.94
-7	43	62	1.19
-5	341	342	-1.14
-3	135	147	0.72
-1	354	345	-1.56
H= 17, K= 1			
0	44	35	-0.80
2	81	87	1.11
4	-28	27	1.68
-6	56	52	-0.67
-4	83	83	-0.52
-2	-26	69	0.60
H= 18, K= 1			
1	240	235	-2.05
3	95	94	2.02
-5	98	101	1.24
-3	286	288	-1.43
-1	148	145	2.02
H= 19, K= 1			
0	73	72	0.99
2	46	57	-1.58
-4	63	66	-2.03
-2	-27	47	-1.30
H= 20, K= 1			
1	185	186	2.05
-3	152	152	1.15
-1	165	185	-1.75
H= 21, K= 1			
0	-30	44	-2.82
-2	61	54	-2.32
H= 0, K= 2			
0	637	589	0.0
2	133	113	-0.75
4	208	205	0.36
6	204	201	2.78
8	213	213	0.18
H= 1, K= 2			
1	382	415	-1.43
3	96	103	2.98
5	116	155	2.61
7	146	152	1.58
9	-27	11	-1.37
-9	-27	12	1.74
-7	-24	26	-0.09
-5	243	250	1.38
-3	214	212	0.64
-1	66	58	-0.29
H= 2, K= 2			
0	167	170	-2.52
2	209	209	-0.88
4	393	410	-2.37
6	78	81	-0.98
8	140	130	-2.83
-8	210	217	-2.85
-5	208	210	0.08
-4	559	577	-3.13
-2	71	75	-2.60
H= 3, K= 2			
1	190	163	-0.86
3	318	331	-1.21
5	81	74	-1.95
7	65	61	-1.66
9	68	70	0.91
-9	124	122	-1.82
-7	74	69	-2.90
-5	-21	31	-0.88
-3	54	63	1.57
-1	377	363	-1.16
H= 4, K= 2			
0	360	346	0.90
2	140	119	2.66
4	104	104	-0.02
6	254	264	-2.69
8	-26	15	1.63
-8	145	150	0.26
-6	315	316	3.11
-4	465	477	0.31
-2	492	514	2.71
H= 5, K= 2			
1	155	187	-1.03
3	270	282	1.83
5	-23	23	2.96
7	47	55	2.99
-9	113	116	1.79
-7	86	86	-1.66
-5	139	136	1.88
-3	164	161	1.05
-1	83	100	1.29
H= 6, K= 2			
0	272	262	1.09
2	555	563	0.47
4	98	94	1.03
6	232	236	0.42
8	45	58	3.04
-8	54	47	-1.24
-6	287	288	-0.27
-4	384	382	-2.92
-2	966	981	0.05
H= 7, K= 2			
1	103	95	-0.12
3	145	149	-1.46
5	219	221	2.02
7	43	32	1.44
-9	61	52	-1.69
-7	214	215	1.82
-5	34	4	2.34
-3	137	143	2.00
-1	126	131	-0.69
H= 8, K= 2			
0	597	563	-0.16
2	191	193	-2.93
4	142	143	-0.49
6	109	121	-2.31
8	109	112	-0.09
-8	37	33	-2.15
-6	213	212	-2.90
-4	112	120	-1.36
-2	816	824	-3.03
H= 9, K= 2			
1	386	395	-1.06
3	128	140	-0.51
5	162	166	-1.39
7	63	72	1.69
-9	95	92	-1.57
-7	180	174	-1.89
-5	321	314	1.99
-3	47	42	-2.33
-1	-21	162	-1.40
H= 10, K= 2			
0	713	686	2.95
2	274	283	0.04
4	208	204	-3.06
6	-26	32	-1.45
-8	102	98	2.45
-6	44	40	2.54
-4	329	319	-3.11
-2	48	51	0.05
H= 11, K= 2			
1	47	37	-0.33
3	145	155	-1.43
5	49	36	2.23
7	83	83	-1.96
-7	78	67	-1.52
-5	110	108	-2.23
-3	510	519	1.86
-1	86	80	1.85
H= 12, K= 2			
0	385	374	0.25

```
   L    FO      FC    ALPHA

   2   298     293     2.41
   4   264     272     0.18
   6    57      64     2.34
  -8   282     280    -0.06
  -6    85      81    -0.42
  -4   120     109    -0.55
  -2   129     135    -2.79

 H=   13,  K=    2

   1    61      56     0.33
   3    45      49     0.94
   5    76      75    -1.93
  -7   101      94    -0.99
  -5    51      48     3.01
  -3    84      85    -2.88
  -1   386     382     1.71

 H=   14,  K=    2

   0   251     250    -2.75
   2   211     211    -0.12
   4   132     131     3.09
  -8   115     107     3.02
  -6   262     262    -0.11
  -4   134     143    -1.83
  -2   121     124    -1.95

 H=   15,  K=    2

   1   187     179     0.95
   3   100     108    -0.62
   5   -29      38     0.47
  -7   -27      48    -1.00
  -5   -26     154    -1.53
  -3   -25     125     2.85
  -1    91      79    -1.57

 H=   16,  K=    2

   0    65      63     2.37
   2   207     217     3.06
   4    78      87     0.07
  -6   158     165     2.77
  -4   -26     217     0.0
  -2   114     120    -2.30

 H=   17,  K=    2

   1   -26      17    -0.06
   3    93      97     1.02
  -5   -27      10    -1.38
  -3   116     120    -2.36
  -1   202     206     2.46

 H=   18,  K=    2

   0   -27      22    -1.42
   2   134     142     1.03
  -6   151     145     0.30
  -4   -27     114     3.10
  -2   229     234    -0.10

 H=   19,  K=    2

   1   139     137     2.21
  -5   109     104    -1.04
  -3    51      49     3.06
  -1   104     109    -2.37

 H=   20,  K=    2

   0   133     124    -0.76
  -4   -28      97    -0.33
  -2   209     207    -2.64

 H=   21,  K=    2

  -3   121     116    -1.56
  -1   -29      42    -2.94
```

```
   L    FC      FC    ALPHA

 H=    0,  K=    3

   1   149     137     2.82
   3   533     530    -1.79
   5   204     205     2.31
   7   182     193    -1.83
   9    77      79     1.51

 H=    1,  K=    3

   0   572     553    -2.77
   2   200     209    -1.96
   4   516     513    -3.01
   6   162     151    -0.06
   8   109     106    -2.57
  -8   139     137     2.28
  -6    88      93     0.41
  -4   271     277     2.86
  -2   609     593    -0.12

 H=    2,  K=    3

   1   203     207     1.34
   3   345     343     1.64
   5   147     148    -1.74
   7   193     191     1.91
   9    59      56    -2.37
  -9   102     101     1.12
  -7   196     204    -1.13
  -5   363     365     1.32
  -3   106     108    -1.34
  -1   893     827     1.40

 H=    3,  K=    3

   0   765     738    -0.14
   2   447     434    -2.88
   4   112     110    -0.12
   6   187     191     2.76
   8   135     128     0.26
  -8   -25      29    -0.88
  -6   173     170     2.12
  -4   399     391     0.10
  -2   133     124     0.76

 H=    4,  K=    3

   1   294     296     0.66
   3   231     219    -1.16
   5   128     124     1.17
   7   160     154    -1.04
  -9    90      88    -1.67
  -7    74      64     1.70
  -5   482     500    -1.58
  -3   314     297     1.44
  -1   419     428    -1.42

 H=    5,  K=    3

   0   148     140     0.53
   2   435     422    -0.21
   4   208     206     3.10
   6   169     166     0.51
   8    96      94     2.13
  -8   191     190    -2.90
  -6    56      62    -1.83
  -4   131     139     1.44
  -2   775     757     0.14

 H=    6,  K=    3

   1   253     245    -1.88
   3    56      65     1.34
   5   188     182    -1.98
   7    98      91     2.45
  -9    52      44     1.99
  -7    88      83    -2.02
  -5   266     261     1.78
  -3   548     542    -1.90
```

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   L    FO      FC    ALPHA

  -1   567     530     1.81

 H=    7,  K=    3

   0   285     284     0.07
   2   439     423    -2.65
   4   189     194    -1.38
   6   197     196    -2.84
   8    56      45    -0.25
  -8    58      53    -0.13
  -6   447     452     3.09
  -4   209     210     2.99
  -2   182     217     2.26

 H=    8,  K=    3

   1   538     519     1.52
   3    37      25    -1.15
   5   118     122     1.43
   7    56      58    -2.40
  -9   -28      30    -1.10
  -7    66      77     0.55
  -5   120     126    -1.17
  -3   460     463     1.44
  -1   381     362    -1.74

 H=    9,  K=    3

   0    97     108     1.37
   2   215     222    -0.13
   4   220     224    -2.68
   6    65      60    -0.59
  -8    40      39    -2.71
  -6   141     143    -0.30
  -4   391     397     2.98
  -2   189     195     1.08

 H=   10,  K=    3

   1   444     425    -1.44
   3   212     215     0.90
   5   129     122    -0.78
   7    85      83     0.37
  -7    68      67    -1.80
  -5   110     115    -1.15
  -3   416     404    -1.59
  -1   281     264     1.29

 H=   11,  K=    3

   0   375     373     0.66
   2   -24      40    -0.23
   4   170     174     0.0
   6    66      76     3.10
  -8   170     179    -0.40
  -6   -24      80    -2.17
  -4   304     309    -0.22
  -2   207     219     2.22

 H=   12,  K=    3

   1   249     243     1.85
   3   223     237    -1.85
   5    60      70     1.61
  -7   211     214     1.65
  -5    95     103     2.28
  -3    68      64    -3.05
  -1   395     386    -2.01

 H=   13,  K=    3

   0   228     234     2.58
   2   117     114     0.24
   4   158     153    -2.03
   6   -28      77    -0.67
  -8   155     144     3.13
  -6    99      96    -1.24
  -4   245     239    -2.87
  -2   197     193     0.0
```

L	FO	FC	ALPHA
H= 14, K= 3			
1	177	184	-2.01
3	224	225	1.67
5	76	74	-2.34
-7	167	165	-1.47
-5	243	246	1.35
-3	193	198	1.52
-1	42	148	1.70
H= 15, K= 3			
0	245	229	0.44
2	-26	139	2.43
4	90	88	0.34
-6	209	208	-2.98
-4	81	90	-1.44
-2	183	175	2.86
H= 16, K= 3			
1	92	79	0.94
3	163	162	-1.35
-7	44	43	0.68
-5	304	306	-1.48
-3	94	86	0.58
-1	89	82	0.61
H= 17, K= 3			
0	142	136	2.23
2	-28	184	0.32
4	49	55	2.37
-6	135	128	-0.48
-4	215	219	-2.81
-2	-26	52	-0.17
H= 18, K= 3			
1	-28	8	2.66
3	81	60	2.21
-5	90	102	1.70
-3	250	251	-1.74
-1	-26	30	3.09
H= 19, K= 3			
0	41	10	2.21
2	-28	87	3.05
-4	121	124	-1.18
-2	253	247	-2.90
H= 20, K= 3			
1	53	50	2.16
-3	169	175	1.53
-1	108	115	-1.83
H= 21, K= 3			
-2	76	87	-0.54
H= 0, K= 4			
0	-21	16	-3.14
2	224	220	0.34
4	285	285	0.34
6	115	111	0.17
8	69	71	0.65
H= 1, K= 4			
1	256	237	-1.63
3	377	384	1.95
5	120	120	-2.18
7	289	273	1.61
9	41	43	-0.68
-9	58	49	0.77
-7	60	60	-1.91
-5	383	521	1.39
-3	252	282	-1.01
-1	123	129	0.05
H= 2, K= 4			
0	248	266	-2.16
2	179	182	-2.50
4	85	93	-1.42
6	125	125	-0.21
8	53	62	-1.03
-8	121	113	2.91
-6	53	61	-2.71
-4	39	41	-1.20
-2	148	154	-1.75
H= 3, K= 4			
1	592	552	-1.37
3	418	415	-1.56
5	173	181	1.72
7	174	171	-1.25
-9	144	152	-1.91
-7	52	54	3.05
-5	215	209	-2.12
-3	533	497	1.52
-1	858	842	-1.40
H= 4, K= 4			
0	322	292	2.81
2	262	265	2.93
4	136	150	2.44
6	94	110	3.12
8	39	12	1.55
-8	58	53	1.10
-6	122	122	2.24
-4	142	149	1.96
-2	112	100	1.81
H= 5, K= 4			
1	443	406	-1.38
3	95	99	-3.03
5	191	188	-2.31
7	190	186	2.00
-9	68	78	1.73
-7	110	109	-1.84
-5	260	274	1.60
-3	38	32	2.76
-1	750	712	1.46
H= 6, K= 4			
0	140	141	-0.99
2	-21	33	1.98
4	70	67	2.02
6	123	110	1.07
8	-27	27	2.66
-8	57	59	-1.00
-6	129	124	-0.19
-4	84	80	-0.35
-2	87	93	0.67
H= 7, K= 4			
1	472	454	1.21
3	181	180	-1.49
5	129	136	2.21
7	88	84	-2.11
-9	81	80	-1.24
-7	124	119	1.67
-5	76	71	-1.84
-3	382	399	1.52
-1	240	241	-0.89
H= 8, K= 4			
0	74	73	-1.80
2	245	240	-1.68
4	81	75	-1.22
6	51	38	-2.16
-8	41	59	-2.67
-6	84	86	-1.88
-4	152	144	-0.25
-2	152	149	-1.37
H= 9, K= 4			
1	551	553	-1.03
3	180	176	0.60
5	167	171	-1.36
7	42	53	1.10
-7	179	169	-1.77
-5	172	168	2.28
-3	-23	236	-1.90
-1	122	122	0.98
H= 10, K= 4			
0	44	35	-2.72
2	90	88	1.96
4	101	103	-2.62
6	-26	24	2.97
-8	70	68	2.56
-6	99	97	2.44
-4	57	53	1.77
-2	259	262	0.65
H= 11, K= 4			
1	207	202	1.56
3	-25	218	-1.34
5	115	129	2.10
-7	90	83	1.68
-5	72	68	-2.98
-3	465	460	1.93
-1	101	97	-2.14
H= 12, K= 4			
0	281	283	0.32
2	73	52	-0.58
4	123	120	0.87
6	-27	17	2.23
-8	103	112	0.06
-6	45	28	-2.52
-4	70	69	2.38
-2	-24	42	1.22
H= 13, K= 4			
1	146	146	-0.80
3	142	134	1.45
5	101	109	-1.44
-7	254	250	-1.41
-5	71	73	2.18
-3	102	100	3.01
-1	418	422	1.69
H= 14, K= 4			
0	157	149	-2.63
2	138	145	-0.45
4	91	92	-1.60
-6	90	81	-0.23
-4	95	89	-2.41
-2	125	136	3.13
H= 15, K= 4			
1	236	230	1.14
3	224	220	-0.78
5	56	50	0.56
-7	79	72	1.10
-5	342	350	-1.58
-3	115	118	-2.72
-1	166	165	-1.84

L	FO	FC	ALPHA
H= 16, K= 4			
0	149	145	2.62
2	168	168	-3.06
4	-28	30	-0.79
-6	108	106	3.07
-4	128	119	0.49
-2	61	56	2.40
H= 17, K= 4			
1	-27	106	-2.15
3	-29	170	1.54
-5	193	195	1.62
-3	191	201	-2.15
-1	157	167	2.67
H= 18, K= 4			
0	54	67	0.46
2	61	69	1.41
-4	51	41	-2.96
-2	176	181	0.31
H= 19, K= 4			
1	-29	111	1.91
-5	125	113	-1.12
-3	228	227	1.79
-1	93	112	-2.45
H= 20, K= 4			
0	105	103	-0.11
-2	85	76	-2.69
H= 0, K= 5			
1	372	358	2.29
3	148	149	2.64
5	72	68	-2.76
7	54	48	-1.52
H= 1, K= 5			
0	692	692	-2.94
2	226	224	-1.51
4	487	484	-2.96
6	230	225	-0.30
8	116	114	-3.05
-8	192	192	2.87
-6	159	163	0.95
-4	608	609	3.07
-2	121	117	-0.12
H= 2, K= 5			
1	166	163	-1.15
3	247	249	1.83
5	85	84	1.20
7	40	30	1.15
-9	72	61	0.77
-7	41	38	0.0
-5	117	122	-0.40
-3	115	122	-1.04
-1	92	99	-0.32
H= 3, K= 5			
0	113	116	0.22
2	523	518	3.14
4	149	149	-0.36
6	277	270	2.96
8	108	101	0.05
-8	140	143	0.30
-6	176	183	2.73
-4	481	488	0.37
-2	563	559	2.99

L	FO	FC	ALPHA
H= 4, K= 5			
1	102	93	1.06
3	141	143	-1.04
5	-25	51	1.33
7	54	66	-0.04
-9	54	47	-2.21
-7	93	91	1.09
-5	64	60	-0.91
-3	320	316	-1.25
-1	277	266	-1.31
H= 5, K= 5			
0	298	292	-3.12
2	231	232	-0.30
4	204	199	2.89
6	243	241	0.08
8	104	98	2.50
-8	154	148	-2.42
-6	266	264	-0.07
-4	48	39	-2.65
-2	952	943	0.06
H= 6, K= 5			
1	202	205	-2.52
3	224	230	2.47
5	98	101	-1.86
7	46	40	-2.37
-9	43	44	1.58
-7	80	77	2.66
-5	199	209	1.67
-3	73	82	-2.95
-1	315	314	-1.87
H= 7, K= 5			
0	634	613	-0.11
2	484	466	-2.82
4	168	171	-1.54
6	205	193	-2.97
-8	-26	30	1.09
-6	365	357	-3.07
-4	219	218	0.30
-2	221	219	3.09
H= 8, K= 5			
1	74	52	-1.60
3	84	86	2.43
5	182	191	1.87
7	-27	15	0.41
-7	93	91	0.87
-5	50	42	0.89
-3	-22	210	0.94
-1	150	125	0.35
H= 9, K= 5			
0	171	160	2.37
2	460	451	0.0
4	236	230	3.07
6	-27	24	-0.35
-8	153	143	-2.91
-6	73	71	0.82
-4	379	370	2.95
-2	472	463	0.40
H= 10, K= 5			
1	113	119	-0.13
3	52	57	-2.21
5	-25	6	-0.85
7	87	84	1.36
-7	62	54	-2.85
-5	61	65	0.84
-3	133	133	-0.99
-1	176	173	-0.09

L	FO	FC	ALPHA
H= 11, K= 5			
0	473	463	0.26
2	81	67	2.60
4	308	306	0.0
6	82	90	2.46
-8	210	216	-0.19
-6	193	203	-2.57
-4	145	147	0.08
-2	279	273	2.80
H= 12, K= 5			
1	70	64	-1.33
3	-25	61	-1.92
5	117	108	-2.49
-7	65	64	2.78
-5	135	127	2.87
-3	-25	50	2.74
-1	156	165	-1.49
H= 13, K= 5			
0	376	365	3.14
2	174	164	-0.53
4	189	183	-2.54
-6	109	121	-0.47
-4	340	338	-2.90
-2	78	74	0.21
H= 14, K= 5			
1	-25	77	-0.70
3	-27	37	1.63
5	-29	23	1.37
-7	-27	1	-0.96
-5	100	113	1.78
-3	63	55	1.41
-1	-26	76	0.41
H= 15, K= 5			
0	238	236	0.48
2	202	204	2.95
4	63	69	-0.24
-6	221	220	-2.91
-4	130	140	-0.10
-2	214	214	2.72
H= 16, K= 5			
1	94	81	-0.16
3	-29	55	-1.06
-5	45	35	3.11
-3	-26	114	1.68
-1	42	101	0.0
H= 17, K= 5			
0	143	151	2.03
2	275	273	0.25
-6	250	243	-0.21
-4	205	217	-2.78
-2	168	165	0.12
H= 18, K= 5			
1	62	57	-0.44
-5	88	89	2.95
-3	103	94	-3.00
-1	87	94	1.96
H= 19, K= 5			
0	54	33	-0.61
-4	164	169	-0.67
-2	303	293	-2.92

```
   L     FO       FC    ALPHA

H=   20,  K=      5

  -3    -29       66     2.36
  -1    -29       10    -2.84

H=    0,  K=      6

   0     56       56     0.0
   2    282      273     2.80
   4     86       85     2.46
   6    129      126     0.38
   8    -26        6    -1.68

H=    1,  K=      6

   1    881      854    -1.53
   3    482      472     1.52
   5    141      140    -1.52
   7    240      243     1.49
  -7    145      153    -1.32
  -5    371      373     1.36
  -3    332      331    -1.13
  -1    535      527     1.21

H=    2,  K=      6

   0    546      526    -2.74
   2    182      185    -0.68
   4     55       51     0.64
   6    -25       39    -1.78
   8     56       53    -0.39
  -8    -27       14    -3.01
  -6     48       41    -1.42
  -4    286      289    -0.56
  -2    241      241    -2.24

H=    3,  K=      6

   1    228      233     1.02
   3    765      743    -1.61
   5    185      184     1.13
   7    188      185    -1.23
  -7    131      132     2.02
  -5    294      304    -1.82
  -3    379      366     1.51
  -1    684      655    -1.46

H=    4,  K=      6

   0    155      146    -3.08
   2    406      385     2.97
   4    118      113     0.83
   6    104      105     1.29
   8     42       43    -2.92
  -8     49       59     1.13
  -6    108      101     0.58
  -4    119      113     0.51
  -2    354      338     0.05

H=    5,  K=      6

   1    309      297    -1.92
   3    391      398     1.82
   5    336      333    -2.13
   7    153      143     1.83
  -7    156      160    -1.82
  -5    365      364     1.69
  -3    114      131    -2.16
  -1    722      712     1.55

H=    6,  K=      6

   0    222      224    -0.54
   2     81       84    -1.48
   4    147      142     2.74
   6     71       62     0.44
  -8     60       64     2.38
  -6     74       76     0.81
  -4    142      141     0.08

   L     FO       FC    ALPHA

  -2     72       58    -2.40

H=    7,  K=      6

   1    596      581     1.34
   3    150      143    -1.69
   5    289      288     1.61
   7    118      111    -2.25
  -7    200      199     1.31
  -5    255      260    -1.55
  -3    411      396     1.35
  -1    220      215    -1.09

H=    8,  K=      6

   0    300      293    -2.53
   2    173      175    -1.02
   4    109      100    -0.58
   6     41       34     2.38
  -8     55       46    -3.00
  -6     73       68     2.50
  -4     88       90     0.31
  -2     85       94    -0.83

H=    9,  K=      6

   1    504      492    -1.34
   3    198      202     0.93
   5    205      207    -1.33
   7     92      103     0.95
  -7    296      295    -1.68
  -5    162      161     1.77
  -3    464      463    -1.72
  -1    144      133     0.75

H=   10,  K=      6

   0    106       94    -3.08
   2    297      298    -3.07
   4    -25       24     2.79
   6    -27       15     1.14
  -8    -28       33     3.12
  -6     84       81     1.12
  -4    168      176     1.12
  -2    124      127     1.07

H=   11,  K=      6

   1    -25      179     1.68
   3    289      289    -1.80
   5    116      125     1.92
  -7    224      225     1.61
  -5    243      246    -1.94
  -3    407      398     1.30
  -1    242      249    -2.06

H=   12,  K=      6

   0     88       81    -0.95
   2     84       90    -2.10
   4    135      142     3.02
   6    -29       19     0.77
  -6     71       65    -3.12
  -4    181      178     0.46
  -2    210      212     0.41

H=   13,  K=      6

   1     86       83    -1.30
   3    193      187     1.37
   5    121      123    -1.78
  -7    138      141    -1.33
  -5    279      280     1.38
  -3    219      219    -1.78
  -1    -27      407     1.50

H=   14,  K=      6

   0    208      204    -0.16
   2    155      142    -1.19

   L     FO       FC    ALPHA

   4    -28       59    -1.59
  -6     79       93    -2.75
  -4     70       68     2.69
  -2    200      204     0.29

H=   15,  K=      6

   1    210      204     1.15
   3    143      142    -1.03
  -5    255      259    -1.65
  -3    168      164     1.39
  -1    -26      299    -1.64

H=   16,  K=      6

   0     93       95     0.69
   2     96       87    -0.07
  -6     75       64    -2.80
  -4    101       93     2.21
  -2    157      160     2.10

H=   17,  K=      6

   1     48      189    -2.02
   3    133      128     1.79
  -5    133      136     1.73
  -3    210      206    -2.05
  -1     51      200     1.75

H=   18,  K=      6

   0     69       68     2.23
   2    -30       36    -0.63
  -4     61       57     2.83
  -2     74       79     1.45

H=   19,  K=      6

  -3    142      139     1.53
  -1    -29      123    -1.83

H=    0,  K=      7

   1    267      276     2.35
   3    280      284     2.00
   5    173      172    -1.54
   7     45       32    -0.14

H=    1,  K=      7

   0    595      584    -3.00
   2    251      243    -0.29
   4    197      199    -2.65
   6    111      109    -0.94
   8    135      138    -2.78
  -8    164      160    -3.03
  -6    111      112     0.31
  -4    231      223    -3.07
  -2     42       43    -1.46

H=    2,  K=      7

   1     76       89     3.08
   3    219      209     1.43
   5    188      185     1.39
   7     95       90    -1.10
  -7     97       98     1.23
  -5    153      168    -0.89
  -3    142      140     0.88
  -1    249      257    -1.64

H=    3,  K=      7

   0    284      287     0.55
   2    404      399     2.88
   4    208      207     0.64
   6    122      125     2.75
   8     43       49     0.44
  -8    156      159     0.30
  -6    130      132     3.01
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```
   L     FO     FC   ALPHA

  -4    311    310    0.46
  -2    150    153    2.35

H=    4, K=     7

   1     79     81    2.96
   3    178    183    2.22
   5    122    117    0.97
   7    106    102    1.31
  -7    -26     12   -1.95
  -5    150    145    0.96
  -3    353    357   -1.23
  -1    161    148    1.11

H=    5, K=     7

   0     60     66   -1.76
   2    424    428    0.10
   4    139    128    3.00
   6    202    194    0.32
  -8    143    138   -2.82
  -6    200    192   -0.20
  -4    197    198   -2.58
  -2    377    370   -0.10

H=    6, K=     7

   1    150    138    2.70
   3    157    155   -3.07
   5     91     92    2.89
   7     54     59   -0.62
  -7    162    161    1.88
  -5     50     58    2.95
  -3     42     43    0.16
  -1    580    568   -1.62

H=    7, K=     7

   0    179    177   -0.83
   2    297    290   -2.63
   4    168    166   -0.28
   6    168    166   -2.65
  -8    104     97    0.13
  -6    298    296   -3.12
  -4    -24     18    0.39
  -2    474    465   -2.93

H=    8, K=     7

   1    451    442   -1.57
   3    104    101    2.08
   5     39     30    2.09
   7    -29     36    1.79
  -7    -26     23   -2.75
  -5    215    220    1.40
  -3    120    112   -0.64
  -1    223    231   -0.41

H=    9, K=     7

   0    363    353    2.92
   2    167    170    0.17
   4    220    205    3.03
   6     85     87    0.72
  -8     66     66    2.83
  -6    299    290    0.22
  -4    226    225    2.81
  -2    155    145    0.90

H=   10, K=     7

   1    107    106    0.06
   3    238    235   -2.00
   5     86     86    2.05
  -7    -26     18    0.50
  -5     59     53    1.88
  -3    283    284    1.19
  -1    141    141   -0.25

H=   11, K=     7
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```
   L     FO     FC   ALPHA

   0    226    223   -0.02
   2    140    137    2.79
   4    239    230    0.02
   6     70     61    2.77
  -6    106    100   -2.55
  -4    -25    425   -0.01
  -2     75     76   -2.71

H=   12, K=     7

   1     40     44   -0.93
   3    -26     16    2.99
   5    163    160   -2.16
  -7     87     85   -3.10
  -5     70     75    2.71
  -3     47     39   -3.09
  -1    180    187    1.13

H=   13, K=     7

   0    181    185   -2.62
   2    135    127   -0.76
   4    163    157   -2.98
  -6     59     52   -0.29
  -4    289    272   -2.97
  -2    252    243   -0.09

H=   14, K=     7

   1    148    150    0.87
   3    -27     23    1.08
  -5     65     63    2.91
  -3    -26     10    0.02
  -1    -26    126   -0.62

H=   15, K=     7

   0    182    175    0.43
   2    115    119    2.92
   4    -29     49    0.22
  -6     58     64    2.56
  -4    -27    141    0.52
  -2    283    275    2.97

H=   16, K=     7

   1    124    132   -0.89
   3     44     47    1.29
  -5     85     80    2.26
  -3     43     45    2.27
  -1    -28     57   -0.15

H=   17, K=     7

   0    160    150   -3.08
   2    -29    164    0.22
  -4    -27     23   -2.65
  -2    199    198    0.11

H=   18, K=     7

   1    -29     42   -0.75
  -3    101    104    2.52
  -1    -28     10    1.14

H=   19, K=     7

  -2    119    119   -2.71

H=    0, K=     8

   0    402    389   -3.14
   2     62     65    1.05
   4    103    101    2.25
   6    112    108   -0.26
   8     56     54   -1.67

H=    1, K=     8
```

```
   L     FO     FC   ALPHA

   1    141    137   -0.08
   3    323    327    1.32
   5     60     62   -0.78
   7    192    191    1.46
  -7    239    244   -1.05
  -5    149    152    1.17
  -3    168    172   -0.68
  -1    476    478    1.30

H=    2, K=     8

   0    123    125   -0.79
   2    204    194   -3.07
   4    151    151    0.29
   6     55     49    1.61
  -8     52     35   -2.27
  -6     59     42    0.21
  -4    173    174   -0.21
  -2    178    175   -2.23

H=    3, K=     8

   1    269    274    1.62
   3    286    282   -1.14
   5     76     76    0.24
   7    133    135   -1.23
  -7    101    102    2.41
  -5    460    459   -1.56
  -3     77     76    2.73
  -1    314    302   -1.70

H=    4, K=     8

   0    257    247   -3.05
   2     96     98    0.64
   4    142    137    2.52
   6     76     81    0.52
  -8     97     85    2.72
  -6    -25     15    1.75
  -4    123    123    0.15
  -2    146    139    0.15

H=    5, K=     8

   1    241    231   -2.43
   3    295    288    2.05
   5    154    157   -1.60
   7    -27     38    2.95
  -7     66     72   -1.82
  -5    229    232    1.93
  -3    458    455   -1.75
  -1    289    292    2.13

H=    6, K=     8

   0     92     89   -1.57
   2    300    295   -2.90
   4     70     66    0.29
   6     61     57    3.00
  -8    107    106    0.33
  -6    108    101    2.68
  -4     45     55    2.97
  -2     89     87   -1.33

H=    7, K=     8

   1    342    329    1.41
   3     79     73   -0.98
   5    232    229    1.51
  -7    219    223    1.20
  -5    173    171   -0.97
  -3    272    269    1.11
  -1    395    387   -1.45

H=    8, K=     8

   0    147    152   -1.55
   2    116    110   -0.60
   4    123    125   -3.13
   6     92     91    0.28
```

L	FO	FC	ALPHA
-6	235	225	0.16
-4	-25	37	0.11
-2	50	46	-2.26
H= 9, K= 8			
1	413	401	-1.77
3	140	134	1.13
5	171	161	-1.06
-7	158	150	-1.73
-5	170	176	1.50
-3	250	251	-1.50
-1	178	169	1.21
H= 10, K= 8			
0	73	83	3.12
2	115	105	-2.53
4	65	66	0.59
6	90	91	2.79
-6	114	121	2.66
-4	360	362	0.32
-2	94	93	0.34
H= 11, K= 8			
1	267	252	1.93
3	284	284	-2.33
5	38	88	1.90
-7	131	120	1.78
-5	-26	156	-1.83
-3	235	236	1.75
-1	137	148	-2.40
H= 12, K= 8			
0	90	89	-1.20
2	-25	90	-2.62
4	98	98	-2.62
-6	47	40	2.43
-4	172	177	2.69
-2	300	301	0.17
H= 13, K= 8			
1	-25	27	-2.24
3	231	229	1.49
-5	145	137	1.07
-3	254	249	-1.06
-1	211	203	1.14
H= 14, K= 8			
0	247	244	-0.13
2	95	92	-1.18
4	-28	17	2.60
-6	128	127	-2.98
-4	74	71	0.89
-2	-26	127	2.65
H= 15, K= 8			
1	56	50	0.23
3	117	112	-1.51
-5	-27	106	-1.60
-3	77	70	0.87
-1	305	307	-1.21
H= 16, K= 8			
0	104	111	2.76
2	122	121	-0.34
-4	141	142	2.65
-2	125	130	0.89
H= 17, K= 8			
1	158	158	-1.65
-3	77	70	-2.03
-1	143	141	1.85

L	FC	FC	ALPHA
H= 18, K= 8			
0	89	94	0.27
-2	123	126	2.56
H= 0, K= 9			
1	347	344	-1.83
3	193	212	1.07
5	125	129	-1.49
7	76	75	2.19
H= 1, K= 9			
0	265	265	-3.00
2	160	167	-0.30
4	153	150	-2.73
6	133	136	-0.51
-6	60	59	-0.88
-4	335	329	-3.11
-2	39	24	-2.14
H= 2, K= 9			
1	328	318	1.72
3	272	268	-1.56
5	101	97	0.93
7	145	139	-1.35
-7	109	107	-0.57
-5	146	144	-1.72
-3	37	43	1.02
-1	406	382	-1.66
H= 3, K= 9			
0	217	207	1.00
2	229	231	2.20
4	143	141	0.86
6	166	169	2.55
-6	43	49	1.68
-4	166	163	0.33
-2	338	341	2.68
H= 4, K= 9			
1	260	243	-1.82
3	366	351	1.73
5	95	94	-1.75
7	69	76	1.22
-7	41	43	2.32
-5	142	145	-0.29
-3	112	111	-1.16
-1	147	151	1.43
H= 5, K= 9			
0	149	139	-2.88
2	285	272	0.06
4	37	39	1.01
6	136	136	0.0
-6	171	173	-0.85
-4	137	129	-2.21
-2	220	215	-0.58
H= 6, K= 9			
1	161	170	1.91
3	209	203	-1.79
5	191	184	1.66
-7	229	231	1.58
-5	81	76	1.87
-3	137	141	-0.91
-1	148	144	-1.39
H= 7, K= 9			
0	108	108	-1.05
2	149	139	-2.89
4	137	133	-0.28

L	FO	FC	ALPHA
6	61	66	-2.21
-6	54	62	-3.10
-4	125	128	-1.54
-2	343	323	-2.78
H= 8, K= 9			
1	141	136	-1.26
3	160	158	1.76
5	125	134	-1.44
-7	193	195	-1.77
-5	246	245	1.53
-3	69	66	0.74
-1	158	155	-1.34
H= 9, K= 9			
0	299	281	2.92
2	137	135	1.19
4	148	144	2.43
-6	213	208	0.40
-4	84	94	1.76
-2	-25	12	1.92
H= 10, K= 9			
1	92	93	-2.80
3	40	50	-1.66
5	149	151	1.90
-7	106	110	1.67
-5	221	233	-1.68
-3	256	250	1.40
-1	100	96	0.72
H= 11, K= 9			
0	103	111	-0.85
2	81	81	-3.11
4	147	146	0.44
-6	-27	26	3.02
-4	229	230	-0.20
-2	75	82	-1.91
H= 12, K= 9			
1	88	75	-0.57
3	110	99	-2.95
-5	163	170	1.68
-3	299	300	-1.57
-1	110	112	1.07
H= 13, K= 9			
0	191	193	-2.40
2	59	60	-1.50
4	88	88	-2.70
-6	53	67	0.15
-4	103	98	-3.05
-2	139	139	-0.97
H= 14, K= 9			
1	68	57	0.52
3	75	87	-0.76
-5	-27	90	-2.15
-3	206	216	1.43
-1	274	270	-1.40
H= 15, K= 9			
0	-27	37	-0.64
2	146	139	3.08
-4	167	165	0.60
-2	107	107	2.09
H= 16, K= 9			
1	143	142	-1.67
-3	-27	43	-2.52
-1	-28	253	1.44

```
   L     FO      FC    ALPHA

 H=   17,  K=    9

   0    -28      45    -2.02
  -2    198     188    -0.08

 H=    0,  K=   10

   0    378     388     3.14
   2     46      44     0.26
   4    223     222     3.12
   6    210     201    -0.24

 H=    1,  K=   10

   1    302     298     1.09
   3    203     211     0.59
   5    174     170    -0.90
   7    -27      23     2.30
  -7    -27      21     0.21
  -5    116     123    -0.66
  -3    221     211    -1.40
  -1    121     126     1.07

 H=    2,  K=   10

   0    183     180     0.08
   2    243     246     3.03
   4    102     101     0.33
   6    135     136     2.94
  -6     70      68     2.75
  -4    367     362     0.03
  -2    150     159    -2.96

 H=    3,  K=   10

   1     35      24     2.16
   3     82      85     0.43
   5    105     106     0.17
  -7     94      92    -0.80
  -5     56      51    -2.93
  -3     95      93    -2.22
  -1    165     156    -2.13

 H=    4,  K=   10

   0    158     156    -3.00
   2    203     200     0.20
   4    142     140     3.09
   6     77      84     0.03
  -6     68      58    -0.16
  -4    117     109    -3.13
  -2    -25     418    -0.10

 H=    5,  K=   10

   1    197     198     2.86
   3     86      86     2.93
   5    -27      40    -2.41
  -7     88      85     1.81
  -5     73      61    -1.38
  -3    133     137     2.43
  -1    267     271     2.65

 H=    6,  K=   10

   0    283     291    -0.22
   2    231     222    -3.11
   4    109     115     0.18
   6     95     102    -2.87
  -6    202     200     3.13
  -4    -25      31     0.65
  -2    229     228    -3.06

 H=    7,  K=   10

   1    223     218     1.90
   3    123     118     1.30
   5     86      89     0.96
  -7    -28      47    -0.15
```

```
   L     FO      FC    ALPHA

  -5    118     113    -0.24
  -3    184     187    -0.99
  -1    155     150     0.91

 H=    8,  K=   10

   0    164     161    -3.10
   2    250     241    -0.07
   4    143     144     2.81
  -6    197     208     0.15
  -4    174     163     3.05
  -2    133     127     0.12

 H=    9,  K=   10

   1     40      40     0.0
   3     67      65     2.43
   5    -30      58    -0.42
  -5    107      97    -1.44
  -3    177     188    -1.23
  -1    235     228    -1.90

 H=   10,  K=   10

   0    145     148    -0.06
   2    137     138    -3.04
   4    145     144    -0.14
  -6    146     141    -3.02
  -4    225     230     0.09
  -2    153     156    -3.12

 H=   11,  K=   10

   1    246     240    -2.75
   3    -26      14    -2.45
  -5    -27      25    -0.26
  -3     63      58    -1.99
  -1    125     129    -1.88

 H=   12,  K=   10

   0    176     174    -3.00
   2     84      89    -0.29
   4    120     130    -2.91
  -4    228     229    -3.11
  -2    168     166    -0.03

 H=   13,  K=   10

   1     47      40    -0.09
   3    117     110     2.66
  -5    143     142     1.11
  -3    142     151    -0.08
  -1     83      83     0.57

 H=   14,  K=   10

   0    182     182     0.03
   2    104      97     2.96
  -4    104     104     0.25
  -2    168     177     3.09

 H=   15,  K=   10

   1    -28      15     2.28
  -3     90      75     0.48
  -1    122     113    -0.99

 H=   16,  K=   10

   0    135     128     3.14
  -2    115     117     0.18

 H=    0,  K=   11

   1    133     128    -1.07
   3    119     123     1.02
   5    276     268    -1.57

 H=    1,  K=   11
```

```
   L     FO      FC    ALPHA

   0     72      74     0.09
   2    -24      26    -2.02
   4    137     132    -2.43
   6    107     107    -1.01
  -6     58      68    -2.39
  -4    252     234    -2.85
  -2     57      45    -1.28

 H=    2,  K=   11

   1     69      65     1.75
   3    154     143    -1.40
   5     85      86     1.47
  -5    269     268    -1.03
  -3    392     385     1.69
  -1     93      93    -1.52

 H=    3,  K=   11

   0    159     163     1.30
   2    215     226     0.83
   4     92      96     1.48
   6    131     130     3.03
  -6    107      99     0.66
  -4     47      41     2.08
  -2    231     303     2.79

 H=    4,  K=   11

   1    -25      21    -2.10
   3    131     133     1.93
   5    -27      56    -1.86
  -5    201     211     1.78
  -3    289     283    -1.65
  -1    493     485     1.64

 H=    5,  K=   11

   0    246     230    -3.14
   2    124     120     0.21
   4    198     205     0.05
  -6    114     119    -0.59
  -4    100      97    -0.99
  -2    102     111    -2.07

 H=    6,  K=   11

   1    317     310     1.34
   3    105     103    -0.93
   5     80      83     1.55
  -5    245     246    -1.36
  -3    214     227     1.56
  -1    379     379    -1.59

 H=    7,  K=   11

   0    108     119    -2.60
   2    204     194     2.99
   4    -27      40    -0.55
  -6    -28      16    -2.23
  -4    107     109    -0.98
  -2    117     123    -1.98

 H=    8,  K=   11

   1    398     390    -1.70
   3    145     142     0.98
   5    131     127    -1.23
  -5    114     116     1.86
  -3    304     303    -1.61
  -1    217     221     1.69

 H=    9,  K=   11

   0     56      61     2.62
   2    134     136     2.16
   4    192     184     2.45
  -6    105      98     0.93
  -4     66      57     1.36
  L     FO      FC    ALPHA

 -2     45      44     0.04

H=  10, K=  11

  1    275     273     1.68
  3    220     215    -1.94
 -5     78      82    -1.30
 -3    240     239     1.65
 -1    206     196    -1.90

H=  11, K=  11

  0    111     107    -0.90
  2     56      56    -0.36
 -4     90      93    -0.46
 -2     94      89    -1.59

H=  12, K=  11

  1    144     144    -1.74
  3    203     206     1.36
 -5     74      71     1.28
 -3    105     114    -1.14
 -1    237     238     1.50

H=  13, K=  11

  0    128     132    -2.20
  2     49      52    -1.70
 -4    -28      26    -0.70
 -2     94      98    -1.26

H=  14, K=  11

  1    142     144     1.61
 -3     49      30     1.91
 -1    153     147    -1.57

H=  15, K=  11

  0    -29      15    -1.45
 -2    -28      36     1.32

H=   0, K=  12

  0    103      97     3.14
  2    163     168    -0.30
  4    320     316    -2.98
  6     94      95    -0.16

H=   1, K=  12

  1    349     358     1.27
  3     76      77     0.56
  5    -27      34     0.49
 -5     84      83    -1.45
 -3     71      79    -0.97
 -1     60      65     0.22

H=   2, K=  12

  0    268     271     0.35
  2     69      73     2.30
  4    162     169     0.11
 -6    132     139     2.96
 -4    227     223     0.15
 -2    247     258     2.82

H=   3, K=  12

  1     89      90    -1.68
  3    187     183     1.12
  5     59      38    -1.27
 -5    -26      14    -2.73
 -3    125     135    -2.17
 -1    143     144    -1.97

H=   4, K=  12

  0    163     165    -3.02
```

```
  L     FO      FC    ALPHA

  2    225     225    -0.11
  4     61      61    -2.36
 -6    116     123    -0.33
 -4    233     241    -3.03
 -2    301     298    -0.17

H=   5, K=  12

  1    157     156    -2.39
  3    146     140    -2.06
  5     63      65     1.22
 -5    -27      35    -2.92
 -3    100     104     2.44
 -1    130     130    -3.04

H=   6, K=  12

  0    259     254     0.01
  2    183     180    -3.12
  4     81      80    -0.49
 -4     87      91     0.06
 -2    324     327     3.05

H=   7, K=  12

  1    117     113     1.16
  3    -26      33    -0.46
 -5    106     110    -0.49
 -3     68      74    -0.45
 -1    154     144     1.40

H=   8, K=  12

  0    251     249     2.70
  2    254     248     0.25
  4    126     112     2.85
 -4    181     178     3.00
 -2    181     184     0.34

H=   9, K=  12

  1    129     117     1.87
  3     76      77     0.99
 -5    -27      43    -0.62
 -3     90      83    -1.32
 -1     67      60    -1.90

H=  10, K=  12

  0    200     205     0.06
  2    130     139     2.87
 -4    154     144    -0.58
 -2    155     200    -2.92

H=  11, K=  12

  1    101      95    -2.72
 -3     52      43    -2.04
 -1     92      97    -2.67

H=  12, K=  12

  0    216     217    -3.10
  2    -28     114     0.17
 -2    102      96    -0.58

H=  13, K=  12

  1    -28      31     2.37
 -3    100      99    -0.05
 -1     48      53    -0.91

H=   0, K=  13

  1    212     222    -1.08
  3    224     232     1.16
  5     69      77    -1.33

H=   1, K=  13
```

```
  L     FO      FC    ALPHA

  0     96     101     0.03
  2     98     104     3.11
  4     73      69    -0.52
 -4     70      67    -1.13
 -2     88      84    -2.97

H=   2, K=  13

  1     63      61     1.16
  3    284     286    -1.61
  5     93      98     1.40
 -5    121     133    -2.14
 -3    149     152     1.95
 -1    267     279    -1.56

H=   3, K=  13

  0    105     106     1.94
  2    117     128     0.52
  4    115     120     2.57
 -4    110     121     2.91
 -2     57      54     0.62

H=   4, K=  13

  1    193     201    -1.55
  3     63      83     1.42
 -5    169     173     1.93
 -3     61      57    -2.86
 -1    272     272     1.68

H=   5, K=  13

  0     49      36    -0.67
  2     37      26     0.85
  4    139     141    -0.25
 -4    155     150    -0.44
 -2    158     165    -2.88

H=   6, K=  13

  1    252     257     1.20
  3    161     158    -1.00
 -5    143     143    -1.29
 -3    189     192     1.58
 -1     40      52    -0.45

H=   7, K=  13

  0    177     179    -3.02
  2    -26      24    -2.75
 -4     64      70    -2.86
 -2    143     136    -0.57

H=   8, K=  13

  1    114     116    -1.68
  3    108     110     1.34
 -3    142     150    -1.98
 -1    197     193     2.02

H=   9, K=  13

  0     91      96     0.18
  2    148     146     2.71
 -4     59      65     0.36
 -2     79      84     2.65

H=  10, K=  13

  1    194     186     1.89
 -3    153     163     2.07
 -1     92      92    -2.50

H=  11, K=  13

  0     44      46    -2.74
 -2    110     112    -0.50
```

```
   L    FO       FC    ALPHA

H=     0,  K=    14

   0   124      126     3.14
   2   183      191    -0.40
   4   156      166    -2.86

H=     1,  K=    14

   1    58       60     0.76
   3    47       66    -0.81
  -3    73       62     0.20
  -1    64       67    -0.92

H=     2,  K=    14

   0   305      307     0.37
   2    99      103     2.71
  -4    77       76     0.89
  -2   150      155     2.31

H=     3,  K=    14

   1    48       52    -1.00
   3    48       48     1.14
  -3    53       54    -1.48
  -1    38       14     0.89

H=     4,  K=    14

   0    92       89    -3.03
```

```
   L    FO       FC    ALPHA

   2   270      269    -0.18
  -4   174      172    -2.77
  -2    55       67    -0.45

H=     5,  K=    14

   1    61       52     2.48
   3    50       23    -2.20
  -3    87      104     1.90
  -1    50       49    -2.03

H=     6,  K=    14

   0    59       67     0.56
   2   133      140     3.12
  -2   201      199     2.98

H=     7,  K=    14

   1    54       62    -0.77
  -3    46       52    -1.09
  -1    68       79     1.47

H=     8,  K=    14

   0   173      166     2.22
  -2   102       95     0.63

H=     9,  K=    14

  -1    85       86    -1.51
```

```
   L    FO       FC    ALPHA

H=     0,  K=    15

   1   165      163    -0.84

H=     1,  K=    15

   0   161      158    -0.20
   2   192      186    -2.96
  -2    78       77     3.10

H=     2,  K=    15

   1    84       79     1.67
  -1    61       54    -1.84

H=     3.  K=    15

   0    91       97     3.05
   2   117      116    -0.09
  -2   127      131     0.12

H=     4,  K=    15

   1   -28       40    -1.69
  -1   108      117     1.85

H=     5,  K=    15

   0   152      156    -0.07
   L     FO       FC    ALPHA

H=     0,  K=     0

   2    213      250     3.04
   4    328      305     0.22
   6    310      306     2.73
   8    315      338     0.41

H=     2,  K=     0

   0    831     1138     3.10
   2   2046     2574    -0.22
   4    682      629    -2.90
   6    141      140    -1.35
   8    235      246    -2.97
  -8    267      296    -3.06
  -6     90       95    -0.49
  -4    905      882     3.13
  -2    170      158    -3.08

H=     4,  K=     0

   0    273      278     1.19
   2   1356     1316     2.95
   4   1138     1067    -0.42
   6    456      449     3.06
  -8    245      258     0.07
  -6    500      479     2.96
  -4    101       97     1.59
  -2    861     1024     2.85

H=     6,  K=     0

   0    362      345     1.65
   2    783      731     0.32
   4    743      686     2.79
   6    609      626    -0.40
  -8    102       99    -2.54
  -6    564      525    -0.33
  -4    411      393    -2.94
  -2    433      507     0.06

H=     8,  K=     0

   0    352      361     0.0
   2    222      208    -3.04
   4    351      347    -0.54
   6    457      496    -3.03
  -8    299      295    -0.04
  -6    417      400    -3.01
  -4    312      319    -0.81
  -2    678      720    -3.02

H=    10,  K=     0

   0    553      528     2.66
   2    451      432     0.46
   4    172      179    -3.02
   6    135      159    -0.52
  -8    236      227     3.07
  -6    462      440     0.02
  -4    529      550    -3.13
  -2    188      193    -0.34

H=    12,  K=     0

   0    458      440     0.30
   2    366      366     1.81
   4    464      504     0.42
  -6    234      232    -3.02
  -4    609      650    -0.27
  -2    336      333    -3.05

H=    14,  K=     0

   0    486      456    -2.96
   2    146      143     0.0
   4    181      184     2.99
  -6    241      235    -0.09
  -4    519      591    -2.96
```

```
   L     FO       FC    ALPHA

  -2    457      460    -0.84

H=    16,  K=     0

   0    250      246    -0.71
   2    338      348     2.82
  -4    253      269    -0.26
  -2    593      594    -3.08

H=    18,  K=     0

   0    343      323     2.91
  -4     35       20     1.12
  -2    437      432    -0.34

H=     0,  K=     1

   1    792      979     1.54
   3    255      250    -1.64
   5    207      202     2.81
   7    291      310    -2.20

H=     1,  K=     1

   0    180      190    -2.63
   2    559      536     2.93
   4    109      102    -1.82
   6     77       68     0.20
   8     52       57     3.00
  -8    126      143     3.03
  -6     64       68     1.49
  -4    183      180     2.69
  -2    187      202    -2.85

H=     2,  K=     1

   1    871     1000    -1.48
   3    801      756     1.35
   5     91       57     1.66
   7    319      336     2.04
  -7    249      255    -1.09
  -5    546      525     1.62
  -3    477      407     1.39
  -1    498      563     1.33

H=     3,  K=     1

   0     73      120    -2.67
   2    515      492    -2.61
   4    402      363     2.61
   6     31       33    -1.31
   8     68       85     0.32
  -8     58       67    -0.13
  -6    163      162     3.01
  -4    148      130     0.37
  -2     97       82     1.23

H=     4,  K=     1

   1    353      280    -0.73
   3   1321     1284    -1.43
   5    285      273     0.56
   7    180      191    -0.74
  -7     77       74    -3.05
  -5    596      571    -1.63
  -3    407      414     1.89
  -1    102      148    -0.68

H=     5,  K=     1

   0    276      238     0.10
   2    151      124    -0.06
   4    314      281    -2.37
   6    229      242     2.13
  -8    124      129    -2.96
  -6    133      137    -0.44
  -4     32       46     2.52
  -2    467      466     0.04

H=     6,  K=     1
```

```
   L     FO       FC    ALPHA

   1     61       26     0.27
   3    149      142     1.60
   5    702      678    -1.81
   7    113      121     2.05
  -7    265      278    -1.72
  -5    289      288     2.27
  -3    305      325    -2.14
  -1    719      819     1.94

H=     7,  K=     1

   0    435      407    -0.18
   2    103      102    -1.76
   4    123      123    -0.34
   6    200      214    -2.16
  -8     88       88    -0.73
  -6    260      248     3.05
  -4     45       59    -0.59
  -2    112      119     1.63

H=     8,  K=     1

   1    787      754     1.67
   3    184      165     0.21
   5    344      330     1.62
   7    229      281    -2.29
  -7    236      218     0.99
  -5    284      277    -1.25
  -3    557      603     1.70
  -1    143      135     2.97

H=     9,  K=     1

   0    181      173     1.18
   2    302      277    -0.31
   4     58       67    -2.24
   6    117      136     0.36
  -8    105      115     0.92
  -6    100       95    -0.66
  -4    276      265     2.93
  -2     58       70     0.72

H=    10,  K=     1

   1    464      424    -1.41
   3    288      282     0.67
   5    348      376    -0.64
  -7    384      370    -1.30
  -5     48       52    -0.71
  -3    461      499    -1.52
  -1    318      323     1.84

H=    11,  K=     1

   0     92       85     1.21
   2     94       93     1.67
   4    149      153    -0.53
   6     35       50    -3.06
  -6     43       45     0.85
  -4     90       94    -0.41
  -2    216      216     2.58

H=    12,  K=     1

   1    449      414     2.02
   3    314      307    -1.76
   5     85       92     1.77
  -7    241      226     1.71
  -5    380      378    -1.47
  -3    237      236     2.20
  -1    305      293    -2.33

H=    13,  K=     1

   0    188      177     2.68
   2     52       49    -2.67
   4     85       91    -2.85
  -6    187      185    -2.78
  -4     66       69    -2.56
```

```
   L    FO     FC   ALPHA

  -2    41     30    0.85

 H=   14,  K=    1

   1   123    116   -3.14
   3   392    394    1.61
  -5   292    301    1.24
  -3   271    279   -1.43
  -1   437    421    1.98

 H=   15,  K=    1

   0   134    122    1.02
   2    72     77    2.16
   4   -17     23   -1.05
  -6    81     77   -0.26
  -4    77     79   -2.71
  -2    44     50   -1.60

 H=   16,  K=    1

   1   164    162    1.71
   3   175    181   -0.76
  -5   335    358   -1.14
  -3   134    146    0.72
  -1   437    403   -1.57

 H=   17,  K=    1

   0    58     52   -0.93
   2   117    126    0.94
  -4    99    100   -0.49
  -2    52     59    0.84

 H=   18,  K=    1

   1   300    302   -2.20
  -3   284    292   -1.49
  -1   190    182    2.12

 H=   19,  K=    1

  -2    59     51   -1.54

 H=    0,  K=    2

   0   529    624    0.0
   2   161    129   -0.89
   4   278    264    0.38
   6   277    272    2.82
   8   278    297    0.11

 H=    1,  K=    2

   1   411    472   -1.43
   3   138    121    3.01
   5   170    162    2.61
   7   216    219    1.41
  -7    33     26    0.25
  -5   322    309    1.45
  -3   229    195    0.40
  -1    72     59   -0.12

 H=    2,  K=    2

   0   170    218   -2.64
   2   267    260   -0.84
   4   538    505   -2.39
   6    82     81   -1.09
   8   198    216   -2.84
  -8   261    287   -2.71
  -6   258    249    0.09
  -4   691    662   -3.11
  -2    85     66   -1.36

 H=    3,  K=    2

   1   199    150   -0.78
   3   435    415   -1.27
   5   112    101   -2.28
```

```
   L    FO     FC   ALPHA

   7    85     83   -1.82
  -7    73     76   -2.99
  -5    38     36   -1.42
  -3    66     73    1.80
  -1   371    431   -1.20

 H=    4,  K=    2

   0   383    392    0.80
   2   140    144    2.75
   4   144    147   -0.06
   6   353    365   -2.73
  -8   178    193    0.28
  -6   394    373   -3.13
  -4   532    516    0.34
  -2   517    558    2.73

 H=    5,  K=    2

   1   209    206   -0.94
   3   375    353    1.80
   5   -19     33   -2.85
   7   116    125    3.00
  -7   119    116   -1.73
  -5   199    186    1.82
  -3   173    152    1.04
  -1   109    146    1.47

 H=    6,  K=    2

   0   266    235    1.21
   2   686    652    0.42
   4   101     93    0.74
   6   315    321    0.29
  -8    55     62   -0.77
  -6   357    343   -0.29
  -4   425    421   -2.89
  -2   883   1036    0.05

 H=    7,  K=    2

   1   100    107    0.33
   3   198    185   -1.35
   5   307    313    1.37
   7    47     58    0.99
  -7   280    267    1.84
  -5   -18     19   -2.10
  -3   166    185    1.89
  -1   142    151   -0.65

 H=    8,  K=    2

   0   648    613   -0.16
   2   262    260   -2.92
   4   190    187   -0.41
   6   194    202   -2.26
  -8    56     68   -2.00
  -6   250    235   -2.85
  -4   135    140   -1.41
  -2   778    869   -3.04

 H=    9,  K=    2

   1   468    444   -1.07
   3   144    146   -0.55
   5   228    235   -1.46
  -7   219    220   -1.79
  -5   365    349    1.98
  -3    84     80   -2.05
  -1   182    144   -1.59

 H=   10,  K=    2

   0   777    742    2.88
   2   389    357    0.13
   4   265    269    3.12
   6    31      4    2.70
  -6    38     45    2.87
  -4   343    347   -3.11
  -2    32     49    0.15
```

```
   L    FO     FC   ALPHA

 H=   11,  K=    2

   1   -18      8   -1.45
   3   199    198   -1.45
   5    84     75    2.50
  -7    90     86   -1.53
  -5   129    122   -2.10
  -3   531    570    1.84
  -1    81     67    2.00

 H=   12,  K=    2

   0   431    407    0.20
   2   375    349    2.35
   4   380    391    0.13
  -6    83     82   -0.37
  -4   122    113   -0.63
  -2   161    164   -2.76

 H=   13,  K=    2

   1    98     88   -0.02
   3    51     46    0.67
   5    87    104   -1.66
  -7   109    103   -0.73
  -5    55     55   -3.05
  -3    89     89   -2.53
  -1   460    440    1.66

 H=   14,  K=    2

   0   328    306   -2.72
   2   248    246   -0.24
   4   181    180   -3.14
  -6   290    282   -0.09
  -4   148    159   -1.91
  -2   138    140   -2.11

 H=   15,  K=    2

   1   239    229    0.96
   3   159    163   -0.64
  -5   158    158   -1.42
  -3   130    137    2.97
  -1   141    114   -1.60

 H=   16,  K=    2

   0   103    100    2.16
   2   264    272    2.95
  -4   239    255    0.04
  -2   121    128   -2.31

 H=   17,  K=    2

   1    29     14   -0.87
  -5   -16      7   -2.63
  -3   111    111   -2.36
  -1   253    250    2.46

 H=   18,  K=    2

   0    47     45   -1.24
  -4    85     86    2.97
  -2   288    282   -0.09

 H=    0,  K=    3

   1   143    139    2.81
   3   631    591   -1.81
   5   289    275    2.23
   7   232    241   -1.96

 H=    1,  K=    3

   0   523    616   -2.84
   2   216    189   -1.76
   4   674    629   -3.03
   6   217    210   -0.14
  L    FO     FC   ALPHA

  8   162    169   -2.55
 -8   193    218    2.30
 -6   116    124    0.37
 -4   370    345    2.89
 -2   630    634   -0.07

H=    2,  K=    3

  1   206    163    1.04
  3   404    354    1.59
  5   201    195   -1.70
  7   272    283    1.81
 -7   234    238   -1.00
 -5   454    422    1.38
 -3   113    139   -1.44
 -1   782    884    1.40

H=    3,  K=    3

  0   696    772   -0.12
  2   513    479   -2.94
  4   163    157    0.0
  6   256    262    2.68
 -8    36     45   -1.09
 -6   237    239    2.11
 -4   493    467    0.14
 -2   133    128    1.41

H=    4,  K=    3

  1   321    312    0.72
  3   306    291   -1.19
  5   138    142    1.09
  7   217    234   -1.12
 -7    70     65    1.56
 -5   576    539   -1.54
 -3   342    318    1.49
 -1   379    438   -1.42

H=    5,  K=    3

  0   130     82    0.95
  2   527    493   -0.24
  4   288    280   -3.12
  6   243    243    0.43
 -8   232    246   -2.81
 -6   117    105   -1.60
 -4   173    153    1.43
 -2   756    828    0.11

H=    6,  K=    3

  1   269    260   -1.87
  3    98     91    1.73
  5   247    244   -2.07
  7   133    152    2.48
 -7   120    121   -2.20
 -5   289    260    1.84
 -3   557    570   -1.89
 -1   558    568    1.80

H=    7,  K=    3

  0   323    310   -0.04
  2   561    515   -2.73
  4   242    243   -1.46
  6   295    320   -2.90
 -8    59     60   -0.44
 -6   543    532    3.12
 -4   234    220   -3.13
 -2   195    227    2.39

H=    8,  K=    3

  1   620    576    1.47
  3    71     70   -0.79
  5   159    159    1.40
 -7   114    110    0.46
 -5   133    130   -1.32
 -3   431    440    1.43

  L    FO     FC   ALPHA

 -1   378    376   -1.72

H=    9,  K=    3

  0   108    110    1.52
  2   285    282   -0.07
  4   302    302   -2.81
  6    55     53   -0.52
 -6   170    159   -0.32
 -4   427    439    2.96
 -2   196    205    0.99

H=   10,  K=    3

  1   500    465   -1.44
  3   259    254    0.85
  5   194    211   -0.81
 -7    98     92   -1.80
 -5   133    124   -1.06
 -3   387    405   -1.64
 -1   264    259    1.25

H=   11,  K=    3

  0   441    413    0.60
  2    82     58   -0.77
  4   245    254   -0.13
 -6    88     78   -2.24
 -4   318    329   -0.24
 -2   213    232    2.22

H=   12,  K=    3

  1   314    293    1.82
  3   277    269   -1.89
  5    91     98    1.77
 -7   252    240    1.68
 -5    99    104    2.41
 -3    79     80    3.00
 -1   392    385   -2.12

H=   13,  K=    3

  0   269    266    2.59
  2   146    148    0.19
  4   246    258   -1.98
 -6   110    110   -1.20
 -4   251    254   -2.92
 -2   207    212   -0.09

H=   14,  K=    3

  1   199    196   -2.18
  3   302    303    1.56
 -5   269    274    1.33
 -3   177    198    1.46
 -1   171    170    1.77

H=   15,  K=    3

  0   311    286    0.44
  2   180    192    2.24
 -6   213    200   -2.98
 -4    67     81   -1.14
 -2   195    185    2.69

H=   16,  K=    3

  1    81     71    1.00
  3   208    216   -1.50
 -5   315    325   -1.44
 -3    94     92    0.69
 -1    94     89    0.40

H=   17,  K=    3

  0   157    161    2.12
  2   246    251    0.30
 -4   211    221   -2.79
 -2    47     64    0.05

  L    FO     FC   ALPHA

H=   18,  K=    3

 -3   275    280   -1.74
 -1    57     58    2.81

H=    0,  K=    4

  0    24     15    0.0
  2   253    218    0.22
  4   329    307    0.26
  6   142    129    0.05
  8    88     91    0.70

H=    1,  K=    4

  1   300    296   -1.53
  3   492    464    1.85
  5   143    133   -1.99
  7   405    410    1.53
 -7    64     73   -1.97
 -5   721    673    1.41
 -3   309    310   -0.97
 -1   158    173    0.53

H=    2,  K=    4

  0   205    226   -2.12
  2   181    161   -2.50
  4   142    118   -1.42
  6   154    160   -0.26
 -8   135    146    3.09
 -6    95     90   -2.62
 -4    40     36   -1.41
 -2   140    128   -1.64

H=    3,  K=    4

  1   602    548   -1.41
  3   562    501   -1.56
  5   245    240    1.73
  7   251    254   -1.26
 -7    43     58   -2.97
 -5   292    274   -2.06
 -3   604    580    1.52
 -1   772    923   -1.40

H=    4,  K=    4

  0   294    268    2.61
  2   264    259    2.85
  4   187    176    2.30
  6   125    121    3.02
 -8    43     54    1.35
 -6   139    135    2.38
 -4   181    170    2.03
 -2   108    118    1.90

H=    5,  K=    4

  1   514    512   -1.45
  3   182    169    3.10
  5   255    255   -2.40
  7   280    304    2.04
 -7   142    136   -1.92
 -5   324    303    1.66
 -3    54     62   -2.36
 -1   707    796    1.47

H=    6,  K=    4

  0   142    138   -1.07
  2    49     43    1.43
  4    59     66    2.22
  6   150    148    1.02
 -8    64     67   -0.68
 -6   133    128   -0.23
 -4    78     72   -0.50
 -2    82     95    1.04
```

L	FO	FC	ALPHA
H= 7, K= 4			
1	555	518	1.18
3	294	273	-1.42
5	180	183	2.23
-7	149	137	1.66
-5	95	87	-1.70
-3	401	421	1.57
-1	272	298	-0.97
H= 8, K= 4			
0	68	55	-2.43
2	290	278	-1.73
4	87	84	-1.45
6	77	76	-2.25
-6	86	85	-1.83
-4	131	135	-0.29
-2	144	149	-1.52
H= 9, K= 4			
1	681	658	-1.08
3	228	220	0.59
5	254	255	-1.38
-7	228	210	-1.84
-5	187	186	2.31
-3	254	269	-1.82
-1	130	154	1.15
H= 10, K= 4			
0	28	42	-2.69
2	146	132	1.78
4	136	135	-2.57
-6	93	88	2.34
-4	46	55	1.83
-2	245	244	0.65
H= 11, K= 4			
1	296	284	1.62
3	297	293	-1.41
5	195	208	2.12
-7	123	123	1.63
-5	108	102	-3.09
-3	473	504	1.94
-1	95	92	-2.18
H= 12, K= 4			
0	312	286	0.24
2	97	96	-0.69
4	164	180	0.85
-6	43	33	-2.15
-4	57	59	2.23
-2	33	26	1.24
H= 13, K= 4			
1	205	202	-0.75
3	197	196	1.35
-5	96	103	1.89
-3	99	110	3.03
-1	466	459	1.66
H= 14, K= 4			
0	183	172	-2.75
2	165	169	-0.56
4	144	157	-1.59
-6	89	85	-0.14
-4	104	102	-2.38
-2	141	143	2.99
H= 15, K= 4			
1	267	259	1.05
3	318	345	-0.84

L	FO	FC	ALPHA
-5	373	395	-1.60
-3	125	126	-2.82
-1	195	133	-1.87
H= 16, K= 4			
0	191	192	2.45
2	206	210	3.04
-4	124	125	0.48
-2	59	56	2.65
H= 17, K= 4			
1	119	112	-2.42
-3	221	231	-2.19
-1	225	226	2.67
H= 18, K= 4			
0	64	71	-0.04
-2	192	193	0.17
H= 0, K= 5			
1	343	358	2.19
3	170	159	2.38
5	101	96	-2.96
7	54	58	-1.44
H= 1, K= 5			
0	641	754	-2.91
2	243	248	-1.37
4	660	595	-3.00
6	298	285	-0.34
-6	189	185	0.97
-4	724	693	3.12
-2	171	197	-0.18
H= 2, K= 5			
1	205	204	-1.24
3	262	237	1.79
5	131	119	1.01
7	30	42	1.15
-7	30	35	0.0
-5	140	138	-0.41
-3	122	108	-1.33
-1	120	128	-0.72
H= 3, K= 5			
0	164	212	0.17
2	593	575	3.13
4	204	191	-0.15
6	375	380	2.81
-8	162	175	0.46
-6	240	241	2.66
-4	592	558	0.39
-2	565	598	3.01
H= 4, K= 5			
1	78	82	0.95
3	177	162	-1.25
5	45	26	1.61
7	85	105	-0.06
-7	101	108	1.07
-5	59	52	-1.05
-3	339	302	-1.21
-1	235	238	-1.39
H= 5, K= 5			
0	322	333	-3.11
2	298	284	-0.28
4	274	258	3.03
6	328	333	0.01
-6	332	306	-0.05
-4	29	37	-3.01

L	FO	FC	ALPHA
-2	893	1022	0.06
H= 6, K= 5			
1	209	190	-2.50
3	248	243	2.34
5	130	126	-1.96
-7	100	104	2.62
-5	229	212	1.68
-3	84	88	3.08
-1	298	303	-1.81
H= 7, K= 5			
0	661	676	-0.12
2	616	579	-2.86
4	213	208	-1.68
6	292	303	-2.92
-6	453	426	-3.00
-4	235	234	0.38
-2	231	260	3.03
H= 8, K= 5			
1	93	71	-1.39
3	106	99	2.17
5	228	247	1.70
-7	106	109	0.85
-5	56	43	1.13
-3	219	218	0.89
-1	163	147	0.48
H= 9, K= 5			
0	187	197	2.30
2	598	553	-0.03
4	319	315	3.01
6	28	30	1.23
-6	80	73	0.90
-4	405	402	2.97
-2	473	517	0.46
H= 10, K= 5			
1	130	121	0.02
3	88	85	-2.46
5	-19	13	-2.77
-7	61	60	-3.07
-5	61	60	0.67
-3	106	110	-1.12
-1	170	173	-0.04
H= 11, K= 5			
0	555	550	0.25
2	67	77	2.71
4	422	430	-0.14
-6	248	228	-2.56
-4	160	162	0.02
-2	281	282	2.84
H= 12, K= 5			
1	84	78	-1.29
3	50	52	-2.08
-5	131	134	2.87
-3	51	50	-3.03
-1	154	156	-1.61
H= 13, K= 5			
0	446	410	3.13
2	211	209	-0.45
4	270	278	-2.59
-6	139	137	-0.56
-4	371	389	-2.90
-2	66	63	0.09

```
   L    FO      FC   ALPHA

 H=   14,  K=    5

   1    96      90   -0.67
   3    41      39    1.03
  -5    66      67    1.82
  -3    36      56    1.25
  -1    72      75    0.13

 H=   15,  K=    5

   0   301     271    0.47
   2   253     244    2.84
  -4   152     155   -0.09
  -2   252     246    2.75

 H=   16,  K=    5

   1    83      86   -0.47
  -3    75      73    1.79
  -1   114     116    0.05

 H=   17,  K=    5

   0   161     156    2.01
  -2   191     187    0.10

 H=    0,  K=    6

   0    67      57    0.0
   2   292     268    2.75
   4   135     121    2.65
   6   162     159    0.26

 H=    1,  K=    6

   1   860     921   -1.55
   3   574     519    1.55
   5   186     174   -1.50
   7   320     325    1.39
  -7   177     178   -1.26
  -5   486     454    1.37
  -3   393     380   -1.10
  -1   511     567    1.18

 H=    2,  K=    6

   0   469     489   -2.72
   2   203     202   -0.67
   4    85      79    0.68
   6    46      45   -2.41
  -6    50      47   -1.02
  -4   336     320   -0.46
  -2   258     253   -2.34

 H=    3,  K=    6

   1   221     233    1.11
   3   939     869   -1.65
   5   236     226    1.22
   7   257     267   -1.26
  -7   156     156    2.01
  -5   363     335   -1.85
  -3   430     414    1.54
  -1   637     722   -1.48

 H=    4,  K=    6

   0   181     183   -3.05
   2   423     379    2.96
   4   132     124    0.67
   6   143     148    1.10
  -6   141     132    0.49
  -4   128     115    0.57
  -2   350     349    0.04

 H=    5,  K=    6

   1   356     346   -1.92
   3   493     469    1.85
```

```
   L    FO      FC   ALPHA

   5   431     426   -2.21
  -7   195     200   -1.90
  -5   459     429    1.69
  -3   124     139   -2.30
  -1   683     756    1.55

 H=    6,  K=    6

   0   226     219   -0.60
   2   128     123   -1.39
   4   177     164    2.70
   6    83      89    0.30
  -6    95      88    1.08
  -4   161     151    0.11
  -2    88      79   -2.81

 H=    7,  K=    6

   1   657     645    1.27
   3   207     195   -1.52
   5   385     390    1.56
  -7   234     224    1.30
  -5   294     281   -1.54
  -3   449     453    1.33
  -1   234     246   -1.08

 H=    8,  K=    6

   0   302     285   -2.68
   2   193     180   -0.97
   4   107     109   -0.83
   6    56      75    2.03
  -6    67      63    2.63
  -4   107      99    0.46
  -2    97     106   -0.57

 H=    9,  K=    6

   1   599     568   -1.38
   3   231     230    0.85
   5   295     306   -1.38
  -7   358     347   -1.71
  -5   182     175    1.86
  -3   463     489   -1.72
  -1   145     149    0.76

 H=   10,  K=    6

   0    75      71    3.12
   2   354     335    3.13
   4    29      26    2.33
  -6    89      86    1.18
  -4   169     170    1.09
  -2   119     132    1.06

 H=   11,  K=    6

   1   231     216    1.66
   3   369     371   -1.88
   5   176     181    2.08
  -5   269     272   -2.01
  -3   422     447    1.79
  -1   249     254   -2.03

 H=   12,  K=    6

   0    95      90   -1.21
   2   111     115   -2.03
   4   184     191    3.01
  -6    61      68   -2.89
  -4   156     164    0.46
  -2   190     197    0.33

 H=   13,  K=    6

   1   132     125   -0.88
   3   228     242    1.20
  -5   280     283    1.35
  -3   208     229   -1.78
  -1   464     468    1.43
```

```
   L    FO      FC   ALPHA

 H=   14,  K=    6

   0   231     222   -0.20
   2   169     173   -1.37
  -4    50      56    2.63
  -2   212     209    0.28

 H=   15,  K=    6

   1   257     252    1.09
  -5   265     272   -1.67
  -3   160     171    1.47
  -1   339     336   -1.71

 H=   16,  K=    6

   0   123     123    0.64
  -4   104     115    2.32
  -2   159     164    1.99

 H=   17,  K=    6

  -1   264     260    1.83

 H=    0,  K=    7

   1   226     224    2.37
   3   352     331    1.86
   5   232     218   -1.54
   7    37      51   -0.46

 H=    1,  K=    7

   0   546     594   -2.95
   2   234     236   -0.40
   4   271     256   -2.62
   6   120     119   -1.11
  -6   127     121    0.50
  -4   269     244   -3.07
  -2    80      84   -1.15

 H=    2,  K=    7

   1    88      90    2.79
   3   236     203    1.32
   5   253     242    1.32
   7   136     148   -1.18
  -7   139     144    1.32
  -5   186     179   -0.90
  -3   162     149    1.05
  -1   290     312   -1.63

 H=    3,  K=    7

   0   283     313    0.47
   2   455     427    2.87
   4   272     248    0.75
   6   150     150    2.66
  -6   174     170    2.88
  -4   380     361    0.57
  -2   161     164    2.32

 H=    4,  K=    7

   1    97      95   -3.07
   3   273     260    2.14
   5   153     150    1.04
  -7    28      25   -1.65
  -5   207     195    1.02
  -3   362     357   -1.20
  -1   198     206    1.30

 H=    5,  K=    7

   0    84      94   -1.66
   2   480     463    0.04
   4   169     155    3.08
   6   253     258    0.32
  -6   248     233   -0.23
  L     FO      FC    ALPHA

 -4    221     208    -2.60
 -2    412     423    -0.04

H=     6, K=     7

  1    169     165     2.40
  3    167     165    -3.02
  5    141     138     2.50
 -7    199     193     1.88
 -5     64      64    -2.67
 -3     74      70     0.23
 -1    553     576    -1.61

H=     7, K=     7

  0    196     199    -0.62
  2    359     348    -2.61
  4    179     174    -0.34
  6    242     250    -2.68
 -6    378     364    -3.06
 -4     33      27     0.26
 -2    441     482    -2.95

H=     8, K=     7

  1    535     502    -1.62
  3    146     137     2.05
  5     40      28     2.01
 -7     57      43    -2.63
 -5    241     237     1.46
 -3    151     150    -1.03
 -1    238     239    -0.47

H=     9, K=     7

  0    374     363     2.88
  2    241     222     0.19
  4    257     260     3.01
 -6    330     308     0.33
 -4    279     277     2.83
 -2    178     181     0.89

H=    10, K=     7

  1    100     103     0.0
  3    319     318    -2.10
  5    134     147     2.10
 -5     59      61     1.97
 -3    298     315     1.24
 -1    145     144    -0.52

H=    11, K=     7

  0    264     257    -0.01
  2    145     132     2.94
  4    313     315    -0.10
 -6    111      98    -2.31
 -4    431     442     0.02
 -2    102     112    -2.77

H=    12, K=     7

  1     89      81    -0.90
  3     28      14    -2.89
 -5     80      74     2.54
 -3     42      24    -2.98
 -1    222     226     1.06

H=    13, K=     7

  0    235     225    -2.67
  2    139     133    -0.86
 -4    285     284    -2.97
 -2    261     261    -0.02

H=    14, K=     7

  1    191     197     0.81
 -5     74      73     2.92
 -3    -19      11     0.50
```

```
  L     FC      FC    ALPHA

 -1    150     146    -0.63

H=    15, K=     7

  0    257     248     0.49
 -4    130     134     0.67
 -2    287     290     2.86

H=    16, K=     7

 -3     54      59     2.40
 -1     44      41    -0.22

H=     0, K=     8

  0    444     500    -3.14
  2     70      67     1.08
  4    136     128     2.44
  6    145     141    -0.37

H=     1, K=     8

  1    141     144    -0.17
  3    360     351     1.32
  5     78      82    -0.51
 -5    200     187     1.22
 -3    188     183    -0.76
 -1    435     485     1.24

H=     2, K=     8

  0    121     133    -0.54
  2    294     267     3.09
  4    228     205     0.41
  6     80      84     1.52
 -6     91      90     0.52
 -4    239     214    -0.11
 -2    187     190    -2.35

H=     3, K=     8

  1    247     256     1.58
  3    340     300    -1.25
  5     65      61    -0.03
 -7    101     102     2.58
 -5    522     493    -1.51
 -3     77      77     2.50
 -1    301     320    -1.63

H=     4, K=     8

  0    279     282    -2.97
  2    140     134     0.46
  4    184     177     2.60
  6    138     135     0.49
 -6    -19      22    -0.32
 -4    164     159     0.06
 -2    184     175     0.02

H=     5, K=     8

  1    244     253    -2.36
  3    352     318     2.05
  5    185     182    -1.80
 -5    260     235     1.98
 -3    451     455    -1.71
 -1    287     298     2.08

H=     6, K=     8

  0    110     103    -1.52
  2    401     374    -2.91
  4     98      97     0.26
 -6    158     148     2.76
 -4     52      44     3.13
 -2     96     108    -1.36

H=     7, K=     8

  1    351     340     1.33
```

```
  L     FU      FC    ALPHA

  3    120     106    -0.91
  5    281     287     1.38
 -5    179     166    -1.03
 -3    276     277     1.04
 -1    398     404    -1.38

H=     8, K=     8

  0    168     173    -1.48
  2    141     126    -0.51
  4    181     183     3.02
 -6    283     276     0.28
 -4     33      24     0.91
 -2     34      25    -1.45

H=     9, K=     8

  1    473     451    -1.78
  3    134     137     1.08
 -5    192     193     1.63
 -3    229     233    -1.61
 -1    165     167     1.14

H=    10, K=     8

  0     70      68     3.10
  2    151     142    -2.32
  4    101      93     0.35
 -6    136     133     2.72
 -4    392     411     0.33
 -2     69      68     0.33

H=    11, K=     8

  1    304     274     1.89
  3    346     350    -2.43
 -5    141     131    -1.89
 -3    267     282     1.78
 -1    131     133    -2.75

H=    12, K=     8

  0    121     109    -1.65
  2    122     125    -2.75
 -4    197     200     2.71
 -2    328     339     0.18

H=    13, K=     8

  1     34      18     1.32
 -3    234     233    -0.99
 -1    251     246     1.17

H=    14, K=     8

  0    323     304    -0.05
  2    111     109    -1.49
 -4     92      95     0.98
 -2    137     142     2.48

H=    15, K=     8

 -3     38      34     0.17
 -1    339     326    -1.26

H=     0, K=     9

  1    358     375    -1.79
  3    292     270     1.60
  5    169     165    -1.26

H=     1, K=     9

  0    223     246    -2.96
  2    160     155    -0.32
  4    184     176    -2.76
  6    160     166    -0.55
 -6     69      62    -1.30
 -4    378     360    -3.08
 -2     43      31    -1.52
```

```
   L     FO       FC    ALPHA

H=     2. K=       9

   1   354      362    1.77
   3   350      324   -1.60
   5   121      112    0.99
  -5   217      208   -1.75
  -3    34       48    0.81
  -1   429      459   -1.71

H=     3, K=       9

   0   207      209    0.96
   2   233      226    2.13
   4   175      172    0.92
   6   205      208    2.76
  -6    87       84    1.17
  -4   176      167    0.51
  -2   323      345    2.08

H=     4. K=       9

   1   284      277   -1.95
   3   478      451    1.75
   5   120      119   -1.79
  -5   190      186   -0.08
  -3   149      138   -1.31
  -1   164      180    1.49

H=     5, K=       9

   0   148      154   -2.70
   2   292      280   -0.02
   4    52       44    0.53
  -6   189      200   -0.97
  -4   117      114   -1.91
  -2   211      211   -0.53

H=     6, K=       9

   1   191      192    1.72
   3   246      228   -1.79
   5   272      276    1.55
  -5    75       77    1.85
  -3   174      170   -0.62
  -1   197      195   -1.37

H=     7, K=       9

   0    99      101   -0.98
   2   175      164   -2.78
   4   127      129   -0.33
  -6    64       68    3.06
  -4   144      146   -1.81
  -2   296      296   -2.72

H=     8, K=       9

   1   204      190   -1.41
   3   190      192    1.74
  -5   297      288    1.56
  -3    39       50    0.33
  -1   169      175   -1.34

H=     9, K=       9

   0   277      260    2.92
   2   176      172    1.15
   4   156      169    2.34
  -4   113      120    1.74
  -2    36       47    2.61

H=    10, K=       9

   1   141      129   -2.89
   3    69       71   -2.13
  -5   219      218   -1.75
  -3   296      308    1.42
  -1    99       89    0.55
```

```
   L     FO       FC    ALPHA

H=    11. K=       9

   0   104      102   -1.06
   2    81       70   -2.68
  -4   221      232   -0.16
  -2    71       76   -1.74

H=    12, K=       9

   1   135      129   -0.66
  -3   288      304   -1.56
  -1   148      147    1.00

H=    13, K=       9

   0   195      198   -2.40
  -4   100       95   -2.96
  -2   128      128   -0.92

H=    14, K=       9

  -3   194      206    1.34
  -1   322      314   -1.43

H=     0. K=      10

   0   401      449    3.14
   2    44       44    0.44
   4   274      252    3.08

H=     1, K=      10

   1   310      314    1.11
   3   214      205    0.40
   5   218      219   -0.96
  -5   138      140   -0.63
  -3   225      226   -1.41
  -1    89       94    0.90

H=     2, K=      10

   0   183      196    0.20
   2   308      291    2.91
   4   163      148    0.53
  -4   480      455    0.05
  -2   160      172   -2.96

H=     3, K=      10

   1    32       28   -3.12
   3   105       97    0.65
   5   115      123   -0.16
  -5    58       51    2.71
  -3    90       87   -2.26
  -1   143      149   -2.23

H=     4. K=      10

   0   186      195   -2.84
   2   226      211    0.17
   4   174      167    3.11
  -4   143      135   -2.99
  -2   457      485   -0.18

H=     5, K=      10

   1   212      215    2.70
   3   101      100    3.04
   5    32       31    2.97
  -5   109      102   -1.44
  -3   156      152    2.19
  -1   247      270    2.59

H=     6, K=      10

   0   288      309   -0.33
   2   313      296   -3.11
   4   113      116    0.29
  -4    47       49    0.68
  -2   274      291   -3.07
```

```
   L     FO       FC    ALPHA

H=     7, K=      10

   1   240      236    1.82
   3   167      171    1.25
  -5   125      120    0.0
  -3   222      220   -1.07
  -1   181      191    0.87

H=     8, K=      10

   0   197      204    3.11
   2   287      271   -0.08
   4   196      201    2.63
  -4   174      169    2.98
  -2   180      185    0.21

H=     9, K=      10

   1    48       51    0.38
   3    89       88    2.57
  -5   120      121   -1.49
  -3   150      162   -1.19
  -1   261      271   -1.95

H=    10, K=      10

   0   219      211   -0.14
   2   183      181   -2.97
  -4   260      264    0.06
  -2   146      145   -2.90

H=    11. K=      10

   1   297      293   -2.73
  -3    85       84   -1.89
  -1   110      116   -1.90

H=    12, K=      10

   0   219      207   -2.84
  -2   175      184   -0.08

H=    13, K=      10

  -1    81       86    0.15

H=     0, K=      11

   1   136      132   -1.16
   3   159      154    0.89
   5   322      302   -1.50

H=     1, K=      11

   0    85      100    0.06
   2    35       40   -3.02
   4   134      122   -2.46
  -4   280      270   -2.81
  -2    56       47   -1.80

H=     2, K=      11

   1    90       86    2.36
   3   182      166   -1.52
  -5   333      324   -1.60
  -3   391      379    1.73
  -1   127      127   -1.60

H=     3, K=      11

   0   139      151    1.51
   2   249      248    0.70
   4   108      108    1.55
  -4    44       48    2.57
  -2   324      332    2.80

H=     4, K=      11

   1   -20       18   -2.37
   L     FO      FC    ALPHA

   3    210     197     2.07
  -5    265     248     1.72
  -3    314     314    -1.64
  -1    454     494     1.66

 H=     5.  K=   11

   0    259     255     3.03
   2    105      97     0.24
   4    278     276    -0.07
  -4    114     111    -0.82
  -2    119     129    -2.21

 H=     6.  K=   11

   1    337     324     1.30
   3    142     135    -0.67
  -3    240     240     1.41
  -1    405     424    -1.56

 H=     7,  K=   11

   0    122     127    -2.64
   2    232     224     2.74
  -4    115     113    -1.02
  -2    102     114    -1.72

 H=     8,  K=   11

   1    484     467    -1.78
   3    132     128     0.97
  -3    313     320    -1.58
  -1    206     214     1.71

 H=     9.  K=   11

   0     41      32     2.60
   2    142     144     2.16
  -4     55      64     0.91
  -2     41      33    -0.35

 H=    10.  K=   11

   1    327     317     1.69
  -3    250     251     1.61
  -1    197     196    -1.82

 H=    11.  K=   11

   0    120     120    -1.20
  -2     97     102    -1.44
```

```
   L     FO      FC    ALPHA

 H=     0.  K=   12

   0    154     157     3.14
   2    150     157    -0.35
   4    366     349    -3.02

 H=     1.  K=   12

   1    385     405     1.27
   3     83      85     0.29
  -3     62      66    -0.90
  -1     44      44    -0.02

 H=     2,  K=   12

   0    267     293     0.46
   2    127     114     2.28
   4    200     192     0.19
  -4    264     251     0.20
  -2    247     250     2.80

 H=     3.  K=   12

   1     90      92    -1.91
   3    256     249     1.07
  -3    154     157    -2.12
  -1    107     114    -2.15

 H=     4.  K=   12

   0    155     166    -2.83
   2    265     252    -0.06
  -4    244     239    -2.94
  -2    311     328    -0.28

 H=     5,  K=   12

   1    146     148    -2.53
   3    163     162    -2.15
  -3    103     110     2.49
  -1    118     138    -2.90

 H=     6.  K=   12

   0    239     240    -0.12
   2    218     208    -3.07
  -2    313     337     3.07

 H=     7.  K=   12
```

```
   L     FO      FC    ALPHA

   1     97     102     1.10
  -3     97      93    -0.93
  -1    147     150     1.47

 H=     8.  K=   12

   0    256     261     2.65
  -2    187     199     0.33

 H=     9.  K=   12

  -1     91      90    -2.08

 H=     0.  K=   13

   1    215     224    -1.05
   3    242     240     1.01

 H=     1.  K=   13

   0    127     145     0.24
   2    101     106     2.76
  -2     89      93     3.11

 H=     2,  K=   13

   1     51      51     1.52
  -3    131     129     2.17
  -1    260     279    -1.59

 H=     3.  K=   13

   0     98     106     2.01
   2    169     177     0.33
  -2     63      55     0.11

 H=     4,  K=   13

   1    186     188    -1.60
  -1    241     254     1.73

 H=     5.  K=   13

   0     34      23    -0.62
  -2    197     213    -2.84

 H=     6.  K=   13

   1    244     245     1.08
```

FIGURE 2

[M(DAPSC)(H_2O)Cl]$^+$ Complex Ions

The Co(II) coordinates were used for this illustration of the atomic numbering scheme and thermal ellipsoids. The Mn(II), Fe(II), and Zn(II) structures are essentially identical. Hydrogen atoms have been omitted for clarity.

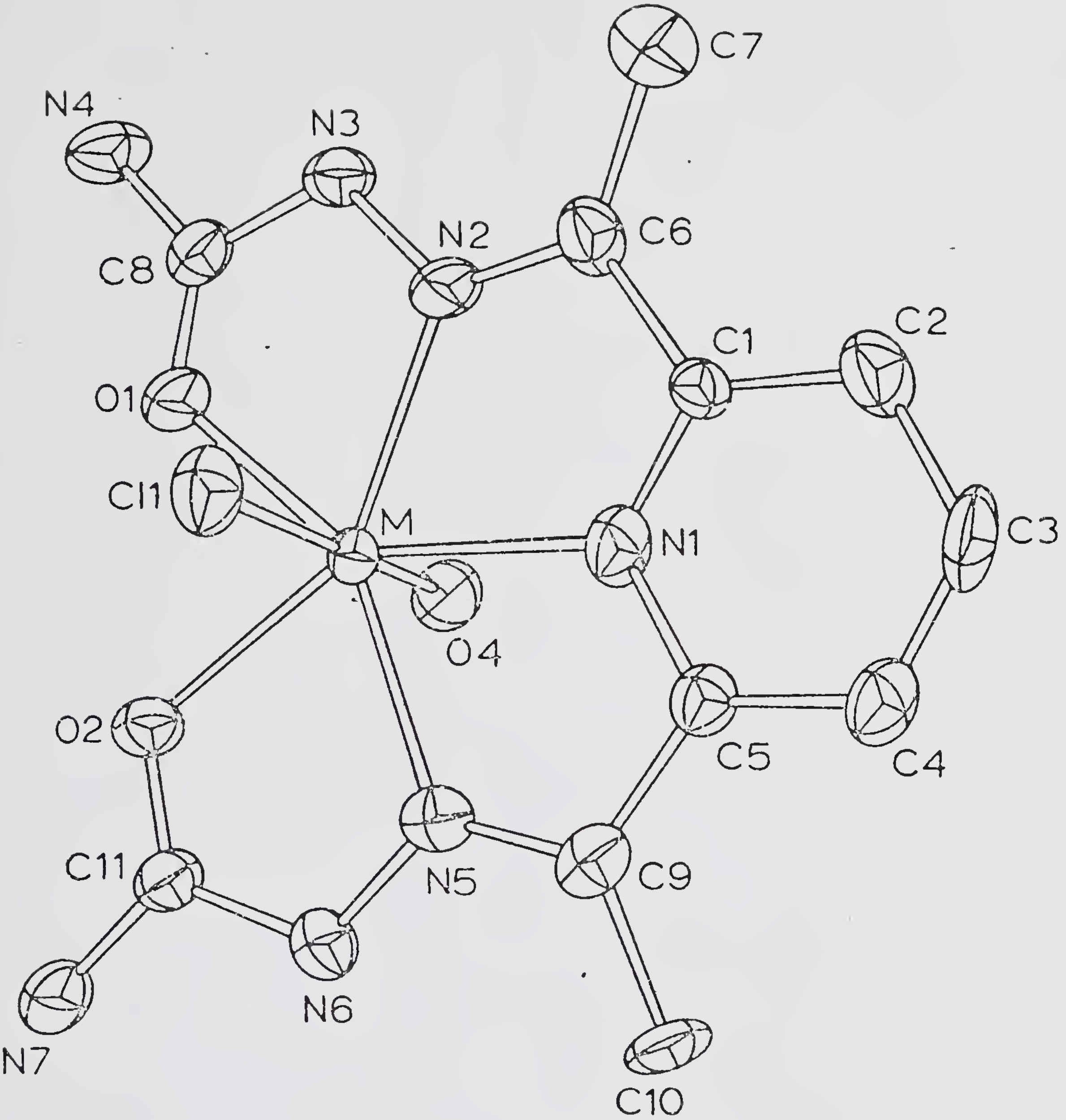
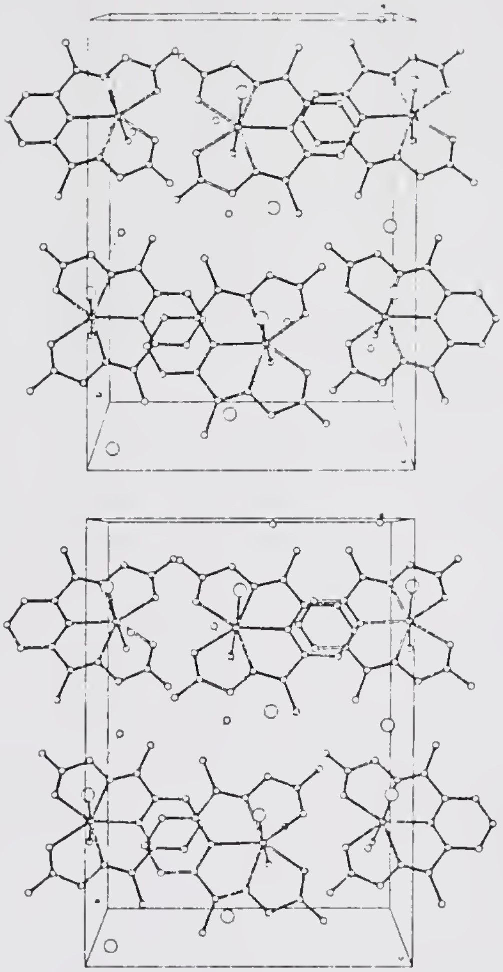

C7
N4
N3
N2
C6
C8
C1
C2
O1
Cl1
M
N1
C3
O4
O2
C5
C4
C11
N5
C9
N6
N7
C10

FIGURE 3

A STEREOSCOPIC PACKING DIAGRAM FOR $[M(DAPSC)(H_2O)Cl]Cl \cdot 2H_2O$

The Co(II) coordinates were used for this illustration of the unit cell contents and packing diagram. The Mn(II), Fe(II), and Zn(II) structures are essentially identical. Larger circles represent chlorine atoms. Dotted lines indicate hydrogen bonds listed in Table 7. Atomic numbering and hydrogen atoms are omitted for clarity.



in general somewhat larger than similar bonds in other complexes of lower coordination number.[23,59-67] This lengthening is certainly a function of many factors. The steric constraints of the DAPSC ligand are most probably the largest contributing factor. The conjugation in DAPSC allows little flexibility except at atoms N3 and N6. Increased donor-donor repulsions are important since an arrangement of five donor atoms in the same plane is much more sterically crowded than the four planar donors in octahedral complexes. The van der Waals radii of O1 and O2 may determine the extent to which these donor atoms approach the metal. The semicarbazone portion of DAPSC can approach the metal ion until the O1-O2 distance is 2.689(9)Å for the Co(II) complex, somewhat less than the sum of van der Waals radii, 2.80Å. The ionic radius of the central metal atom is also a determining factor of the metal-ligand distance. Both the average M-N and M-O distances follow the same trend as the ionic radii of the metals. Thus the shortest distances are associated with the Co(II) complex, while the longest distances occur in the Mn(II) species. These trends are portrayed graphically in Figures 4 and 5.

The metal-chloride and metal-water bonds are also expectedly longer than corresponding bonds in other complexes.[66-72] However, the bond distances decrease on going from Mn(II) to Zn(II), Figure 5. Consideration of the orientation of orbitals into which added electrons are placed, the ionic radius of the metal and non-bonded contacts provide an explanation for this phenomenon. If the high

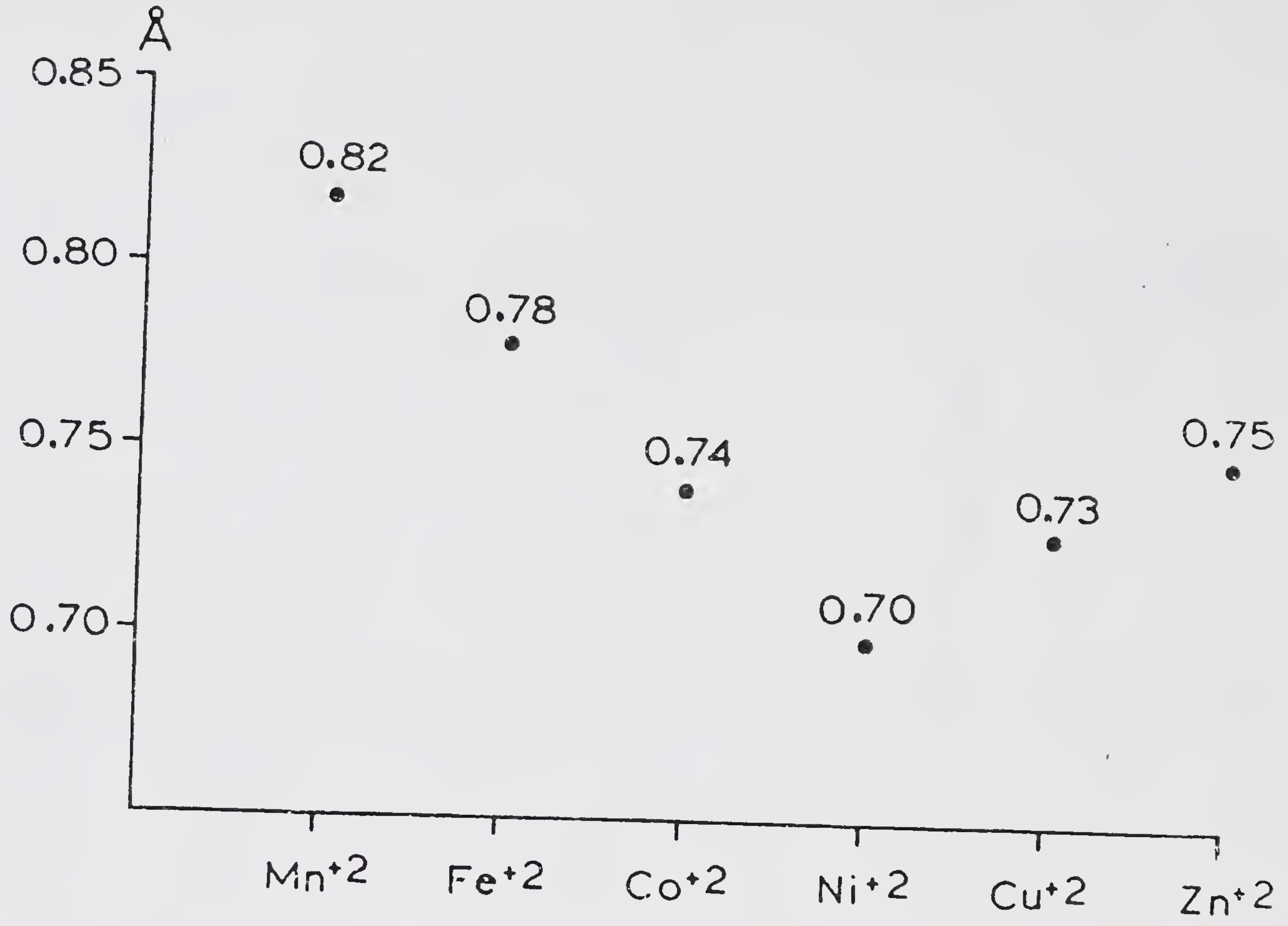


FIGURE 4. IONIC RADII OF THE LATTER FIRST-ROW TRANSITION METAL (II) IONS, AS DETERMINED BY SHANNON AND PREWITT.

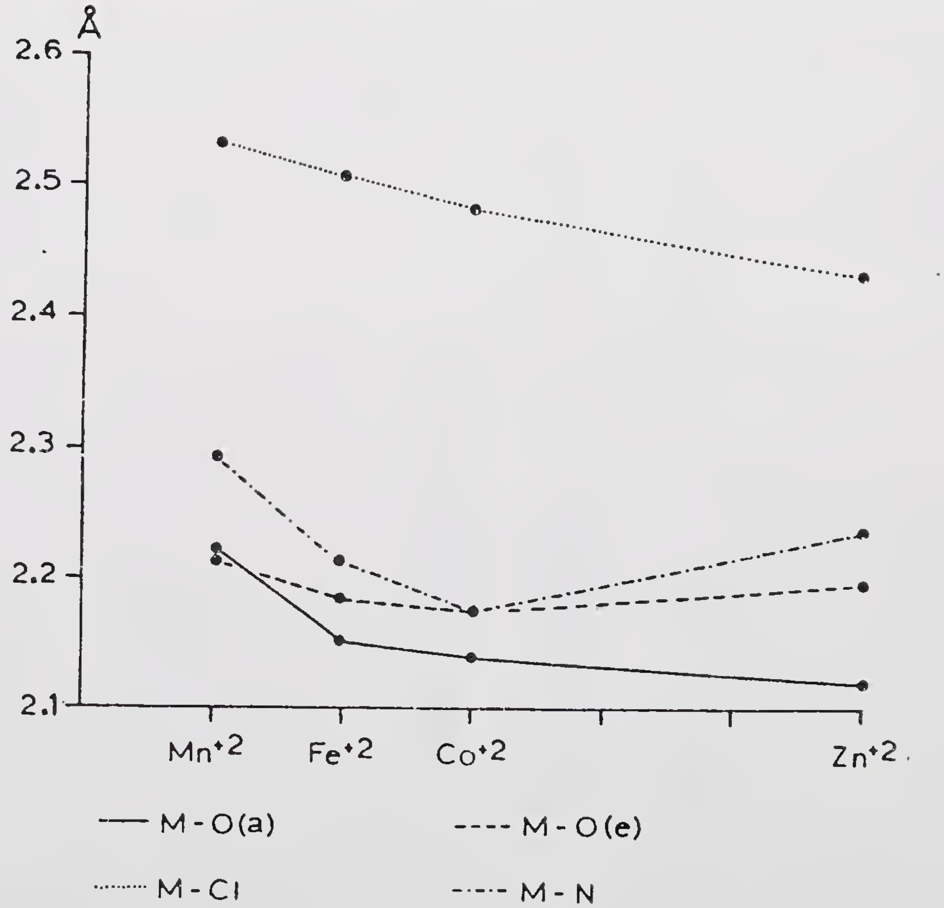


FIGURE 5. METAL-LIGAND DISTANCES FOR $[M(DAPSC)(H_2O)Cl]^+$ IONS

Trends in the metal-ligand distances in the complex ions going from Mn(II) to Zn(II) are depicted accoridng to the legend. Data for the Ni^{+2} and Cu^{+2} complexes are not available.

spin Mn(II), d^5, is taken as a starting point, the next electron added would enter an orbital directed between the ligands (dxy, dyz). Thus Fe(II), d^6, which also has a smaller ionic radius than Mn(II) would exhibit shorter bonds as is the case. Similarly, Co(II), d^7, places the added d electron in an orbital directed between the ligands and has a still smaller ionic radius than Fe(II), so that the Co(II) bond distances are predictably less than those for Fe(II). When the d^{10}, Zn(II), configuration is attained, one electron has been added into each of the $d_{x^2-y^2}$ and d_{xz} orbitals directed at the planar ligands and one into the d_{z^2} orbital directed at the axial ligands. Thus the metal-DAPSC distances increase as a result of electron-electron interactions. Although the ionic radius of Zn(II) is very close to that of Co(II), the metal-axial donor distances decrease. This suggests that these distances are determined by non-bonded contacts with the planar donors. Indeed, the non-bonded contacts are not significantly different for Co(II) or Zn(II) and are only slightly larger than the sum of van der Waals radii, as shown in Table 10.

The bond distances in DAPSC are similar to those previously reported for similar species.[23,66,67,73] The deviations of the donor atoms from planarity are significant, indicating that the ligand does possess some flexibility. The arrangement of the donors about the metal can be interpreted in two ways. If the plane through the donor atoms is considered, the resulting arrangement places N1 nearly

Table 10
NON-BONDED CONTACTS IN $[M(DAPSC)(H_2O)Cl]^+$

The contact distances (Å) between the atoms listed at the left are given below the appropriate metal symbol. Respective estimated standard deviations are in parentheses. The designations (e) and (a) refer to equatorial and axial donors respectively.

	M=Mn	Fe	Co	Zn	Sum of van der Waals radii
Cℓ-O(e)	3.46(1)Å	3.38(1)Å	3.34(3)Å	3.34(2)Å	3.20Å
Cℓ-N(e)	3.45(8)	3.35(8)	3.31(8)	3.34(7)	3.30
O(a)-O(e)	3.02(4)	2.96(4)	2.93(6)	2.92(6)	2.80
O(a)-N(e)	3.18(7)	3.12(6)	3.10(6)	3.10(6)	2.90
O(e)-O(e) (O1-O2)	2.955(11)	2.761(8)	2.689(9)	2.777(13)	2.80

Table 11
STACKING DATA FOR PYRIDINE RINGS

The distances (Å) are given for the metals listed on the left. Angles are in degrees and decimal fractions. Respective estimated standard deviations are in parentheses.

	Mid-Point - Mid-Point Dist.	Mean Deviation	Angle
Mn	4.095	3.46(1)	1.77
Fe	4.069	3.42(1)	1.90
Co	4.071	3.43(1)	1.93
Zn	4.072	3.43(1)	1.62

on the plane with O1 and N5 below and O2 and N2 above the plane. Such an arrangement has been designated puckered coordination.[23] However, if the plane through the pyridine ring is considered, the resulting arrangement has O1 and N2 below and O2 and N5 above the plane with N1 on the plane. Such a conformation of the ligand has been called helical.[23] The dihedral angle of ~6° between these planes can be shown to be responsible for the different conformations.

The packing of the unit cell is characterized by hydrophilic and hydrophobic interactions.

The hydrogen bonding interactions (hydrophilic) are listed in Table 7. Both water and chloride of the complex ion and lattice participate in the bonding pattern. All distances between hydrogen bonded atoms are less than the sum of van der Waals radii and below the limit within which hydrogen bonds are said to exist.[74,75] The apical water, O4, is hydrogen bonded to the ionic chloride, Cℓ2, and a lattice water, O3. The apical chloride, Cℓ1, hydrogen bonds to two lattice waters, O5 and O3. Additional hydrogen bonds involving the semicarbazone NH's (N3-H with Cℓ2 and N6-H with O5) and ionic chloride (Cℓ2 with lattice water O5) are also present.

The outstanding feature of the hydrophobic interactions is the stacking of the pyridine rings. Data pertaining to this stacking appear in Table 11. Because the pyridine rings are not stacked directly above one another, the distance from mid-point to mid-point is larger than the mean deviation of atoms from the plane of one ring with respect to its neighboring ring. The mean deviations may vary from 3.42(1)Å to 3.46(1)Å. This distance is considerably shorter than the separation observed in other pyridine,* phenyl,[76] and tropolonate[77] stacking arrangements. The dihedral angle between the rings is less than 2° for all compounds, indicating a high degree of coplanarity.

In conclusion, these complexes present the first opportunity to systematically investigate the structural characteristics of pentagonal bipyramidal complexes of first-row transition metals. The planar donors are primarily influenced by the ionic radius of the metal ion. Steric crowding of the five donors seems to be a minor factor, suggesting that the other planar pentadentate ligands may be useful in forming pentagonal bipyramidal complexes. The axial donors appear to be influenced by non-bonded contacts,[78] providing the ionic radius of the metal is small enough to allow such steric interactions to occur. In general, the final geometry of a metal complex demonstrably depends upon the constraints of the ligand.[56,79]

Structure Solution and Refinement for $[Fe(DAPSC)Cl_2]Cl \cdot 2H_2O$

The iron atom position was estimated from a sharpened three-dimensional Patterson function. A Fourier synthesis phased on this atom established the position of two chlorine atoms. Another Fourier synthesis using these three atoms sufficed to locate all non-hydrogen atoms in the structure. A difference Fourier synthesis revealed no additional atoms, R=0.20. Three cycles of least-squares refinement with individual isotropic thermal parameters reduced R to 0.11. Conversion to anisotropic thermal parameters followed by six least-squares cycles refined the structure, R=0.056. A difference Fourier synthesis revealed the positions of all hydrogen atoms in the structure. The hydrogens were assigned isotropic thermal parameters one unit larger than the refined isotropic thermal parameter of the bonded atom. Three cycles of least-squares refinement of the non-hydrogen atoms using anisotropic thermal parameters reduced R to 0.048. The shifts of all parameters were less than one-tenth of their respective estimated standard deviations. Refinement was terminated.

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* W. L. Steffen, private communication

Results for $[Fe(DAPSC)Cl_2]Cl\cdot 2H_2O$

The final positional and thermal parameters for the non-hydrogen atoms are listed in Table 12. The probable positional parameters and bond distances for the hydrogen atoms appear in Table 13. Intramolecular bond distances and angles, and short intermolecular contacts are given in Table 14. Least-squares planes and deviations are tabulated in Table 15. The observed and calculated structure factors are in Table 16. Figure 6 is an ORTEP[58] drawing of the complex ion illustrating the atomic numbering scheme. An ORTEP[58] packing diagram of the unit cell contents

Table 12
FINAL POSITIONAL AND THERMAL PARAMETERS ($\times 10^4$) FOR THE NON-HYDROGEN ATOMS OF
$[Fe(DAPSC)Cl_2]Cl \cdot 2H_2O$
WITH THEIR RESPECTIVE ESTIMATED STANDARD DEVIATIONS IN PARENTHESES

Atom	X	Y	Z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Fe	1641(1)	1290(1)	3370(1)	30(1)	46(1)	22(1)	4(1)	29(1)	0(1)
Cℓ1	1676(1)	3096(1)	3164(1)	74(2)	47(1)	39(1)	5(2)	65(2)	-3(2)
Cℓ2	1526(1)	-501(1)	3366(1)	52(1)	48(1)	39(1)	5(2)	52(2)	8(2)
Cℓ3	6810(1)	1459(2)	3668(1)	51(1)	108(2)	70(1)	4(3)	81(2)	28(3)
O1	1382(3)	1397(3)	4741(3)	39(4)	67(3)	30(3)	8(6)	36(5)	3(5)
O2	3448(3)	1304(3)	4678(3)	39(4)	70(3)	32(3)	8(6)	36(5)	0(5)
N1	570(4)	1252(4)	1592(3)	51(5)	40(3)	31(3)	11(7)	47(6)	7(6)
N2	-378(4)	1316(4)	2804(3)	40(4)	48(4)	32(3)	5(6)	43(6)	3(6)
N3	-701(4)	1296(4)	3591(4)	44(5)	66(4)	35(3)	8(7)	50(7)	0(6)
N4	69(5)	1269(4)	5427(4)	72(5)	59(4)	37(3)	-4(7)	75(7)	3(6)
N5	2929(4)	1207(4)	2718(4)	40(4)	45(4)	37(3)	-2(7)	40(6)	-4(6)
N6	4155(4)	1213(4)	3487(4)	43(4)	59(4)	47(4)	-4(7)	54(7)	-3(6)
N7	5538(4)	1271(5)	5317(4)	32(5)	74(4)	56(4)	11(7)	35(7)	2(7)
C1	-675(5)	1275(5)	1072(4)	41(5)	40(4)	26(4)	5(8)	20(7)	2(7)
C2	-1375(6)	1272(5)	-48(5)	55(6)	50(4)	33(4)	7(9)	27(8)	6(7)
C3	-780(6)	1252(5)	-640(5)	84(7)	42(4)	27(4)	-4(9)	34(8)	1(7)
C4	529(6)	1232(5)	-99(5)	89(7)	35(4)	36(4)	1(9)	71(9)	5(7)
C5	1180(5)	1235(4)	1020(4)	55(5)	33(4)	34(4)	-5(8)	54(8)	-1(6)
C6	-1222(5)	1296(5)	1793(5)	44(5)	48(4)	38(4)	14(8)	37(8)	6(7)
C7	-2599(6)	1270(7)	1360(5)	40(5)	145(9)	44(5)	16(11)	24(9)	-18(11)
C8	321(5)	1322(4)	4622(4)	52(5)	34(4)	35(4)	-1(8)	50(7)	1(6)

Table 12 - continued

Atom	X	Y	Z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
C9	2556(6)	1223(5)	1697(5)	70(6)	38(4)	40(4)	-8(8)	76(9)	-2(7)
C10	3387(6)	1238(6)	1214(6)	82(7)	89(6)	56(5)	14(12)	107(11)	6(10)
C11	4363(5)	1265(5)	4521(4)	45(5)	43(4)	46(4)	5(8)	48(8)	8(7)
O3	5976(5)	3662(5)	2507(4)	104(5)	114(6)	72(4)	-13(9)	58(8)	32(8)
O4	3465(6)	4052(7)	1896(5)	130(6)	214(10)	111(6)	-13(13)	82(10)	-72(12)

Table 13

POSITIONAL AND THERMAL PARAMETERS (x 10^3) FOR THE HYDROGEN ATOMS OF $[Fe(DAPSC)Cl_2]Cl \cdot 2H_2O$

ATOM	BONDED TO	DISTANCE,Å	X	Y	Z	B($Å^2$)
H1	N3	0.97	-159	133	337	3.5
H2	N4	0.86	66	129	609	3.6
H3	N4	0.90	-67	118	541	3.6
H4	N6	1.00	488	130	336	3.6
H5	N7	0.97	576	130	608	4.2
H6	N7	0.84	618	121	524	4.2
H7	C2	0.91	-223	126	-41	3.7
H8	C3	1.01	-122	120	-146	3.9
H9	C4	0.97	79	129	-64	3.8
H10	C7	0.92	-268	101	193	5.5
H11	C7	0.92	-286	184	158	5.5
H12	C7	0.93	-316	96	70	5.5
H13	C10	1.10	436	143	180	4.8
H14	C10	1.08	376	48	121	4.8
H15	C10	0.92	315	133	49	4.8
H16	O3	0.79	526	373	235	6.6
H17	O3	1.09	623	289	287	6.6
H18	O4	1.17	401	420	284	9.5
H19	O4	1.07	349	323	201	9.5

Table 14
INTRAMOLECULAR BOND DISTANCES AND ANGLES AND SHORT INTERMOLECULAR CONTACTS FOR
[Fe(DAPSC)Cl$_2$]Cl·2H$_2$O
WITH THEIR ESTIMATED STANDARD DEVIATIONS IN PARENTHESES

(a) Bond Distances (Å)

Fe-Cℓ1	2.362(2)	N4-C8	1.328(8)
Fe-Cℓ2	2.325(2)	N5-N6	1.355(7)
Fe-O1	2.131(4)	N5-C9	1.288(7)
Fe-O2	2.074(4)	N6-C11	1.364(7)
Fe-N1	2.196(4)	N7-C11	1.321(8)
Fe-N2	2.200(5)	C1-C2	1.385(8)
Fe-N5	2.203(6)	C1-C6	1.481(9)
O1-C8	1.236(8)	C2-C3	1.363(10)
O2-C11	1.254(8)	C3-C4	1.400(10)
N1-C1	1.331(8)	C4-C5	1.381(8)
N1-C5	1.355(8)	C5-C9	1.476(10)
N2-N3	1.362(7)	C6-C7	1.489(10)
N2-C6	1.290(7)	C9-C10	1.488(11)
N3-C8	1.379(7)		

(b) Bond Angles (°)

Cℓ1-Fe-Cℓ2	173.6(1)	N3-N2-C6	120.9(5)
Cℓ1-Fe-O1	94.0(1)	N2-N3-C8	112.9(5)
Cℓ1-Fe-O2	91.4(1)	Fe-N5-N6	114.0(4)
Cℓ1-Fe-N1	85.2(1)	Fe-N5-C9	123.2(4)
Cℓ1-Fe-N2	91.5(1)	N6-N5-C9	122.7(5)
Cℓ1-Fe-N5	86.2(1)	N5-N6-C11	114.0(5)
Cℓ2-Fe-O1	91.8(1)	N1-C1-C2	121.7(6)
Cℓ2-Fe-O2	92.8(1)	N1-C1-C6	114.3(5)
Cℓ2-Fe-N1	88.5(1)	C2-C1-C6	124.0(6)
Cℓ2-Fe-N2	87.6(1)	C2-C1-C6	124.0(6)
Cℓ2-Fe-N5	90.4(1)	C1-C2-C3	119.5(6)
O1-Fe-O2	76.1(2)	C2-C3-C4	119.2(6)

Table 14 - continued

(b) continued

O1-Fe-N1	141.1(2)	C3-C4-C5	118.9(6)
O1-Fe-N2	71.2(2)	N1-C5-C4	121.0(6)
O1-Fe-N5	148.8(2)	N1-C5-C9	114.1(5)
O2-Fe-N1	142.7(2)	C4-C5-C9	124.9(6)
O2-Fe-N2	147.4(2)	N2-C6-C1	112.3(5)
O2-Fe-N5	72.6(2)	N2-C6-C7	125.7(6)
N1-Fe-N2	69.9(2)	C1-C6-C7	122.0(6)
N1-Fe-N5	70.1(2)	O1-C8-N3	119.4(5)
N2-Fe-N5	140.0(2)	O1-C8-N4	124.8(6)
Fe-O1-C8	119.9(4)	N3-C8-N4	115.8(5)
Fe-O2-C11	119.9(4)	N5-C9-C5	112.7(6)
Fe-N1-C1	120.3(4)	N5-C9-C10	125.4(6)
Fe-N1-C5	119.9(4)	C5-C9-C10	121.9(6)
C1-N1-C5	119.8(4)	O2-C11-N6	119.4(6)
Fe-N2-N3	116.0(4)	O2-C11-N7	123.0(6)
Fe-N2-C6	123.1(4)	N6-C11-N7	117.6(6)

(c) Short Intermolecular Contacts (Å)

ATOM A	EQUIV. POS.	ATOM B	EQUIV. POS.	DIST.
Cℓ3	X,Y,Z	O3	X,Y,Z	3.201(7)
O3	X,Y,Z	O4	X,Y,Z	2.812(10)
O4	X,Y,Z	Cℓ3	1-X,½+Y,½-Z	3.197(10)
N3	1+X,Y,Z	Cℓ3	X,Y,Z	3.128(6)
O4	X,Y,Z	O1	X,½-Y,Z-½	2.914(8)
O4	X,Y,Z	O2	X,½-Y,Z-½	3.178(8)
O3	X,Y,Z	N7	X,½-Y,Z-½	2.887(7)

Table 15
LEAST-SQUARES PLANES AND DEVIATIONS FOR $[\mathrm{Fe(DAPSC)Cl_2}]\mathrm{Cl}\cdot 2\mathrm{H_2O}$

The title and equation of the plane are given followed by selected atoms and their deviations (x 10^3 Å). Equations are of the form ax+by+cz=d, where d is the distance (Å) from the origin. Atoms used to define the plane are designated by an asterisk. Dihedral angles between planes are given in degrees and decimal fractions.

Plane 1. Plane Through Pentagonal Donor Set

$0.0366x + 0.9986y - 0.0379z = 1.5078$

Fe	-10	O2*	-4
Cℓ1	2344	N1*	23
Cℓ2	-2332	N2*	-25
O1*	18	N5*	-11

Plane 2. Plane Through the Pyridine Ring

$0.0220x + 0.9998y - 0.0017z = 1.6124$

Fe	44	C1*	2
O1	151	C2*	0
O2	88	C3*	0
N1*	-2	C4*	0
N2	33	C5*	2
N5	-17		

Dihedral angle between Planes 1 and 2 = 2.23

Table 16

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $[Fe(DAPSC)Cl_2]Cl \cdot 2H_2O$

The structure factors for the reflection (HKL) are listed to the right of the appropriate L value under the corresponding H and K values. FO and FC refer to F_{obs} and F_{calc} respectively.

```
   L    FO     FC       L    FO     FC       L    FO     FC       L    FO     FC

                       6   -37    -43       0   164   -185      10   147    164
H=   0, K=      0      8   785   -797     -12   205    208      11   429    442
                     -14   332    385     -10   315   -326     -14   250    254
   2   624   -701    -12   216    213      -8    80     86     -13   412    419
   4   942   -877    -10  1238  -1277      -6   -37     26     -12   103   -124
   6  2021   2022     -8   507    495      -4   190   -194     -11   307   -307
   8   180   -178     -6   913    843      -2   483    506     -10   -34     29
  10   716   -704     -4  1021   -977                            -9   -33    -15
  12   379    357     -2   498    559    H=  12, K=      0      -8   297    286
                                                                -7   737    797
H=   1, K=      0    H=   6, K=      0     -12   483    470      -6   479   -463
                                          -10   746   -753      -5  1059  -1014
   0  1699   1840      0  1135   1175      -8   285   -289      -4    89     24
   2   993   1036      2   645   -613      -6   724    702      -3   116   -171
   4  1161  -1195      4    51     44      -4   737   -737      -2   718    733
   6  1522   1445      6   477    488      -2   285   -280      -1   507    378
   8   461    442      8   353   -365
  10   455   -438    -14   118   -141    H=  13, K=      0    H=   3, K=      1
  12   394    419    -12    89     53
 -12   224    242    -10   371   -356     -10   161    186       0   -34     54
 -10   451    453     -8   260   -253      -8   244   -240       1   222   -199
  -8  1288  -1331     -6  1892   1889      -6   379    394       2   941   -872
  -6   188    140     -4   924   -997                             3   878   -882
  -4   523    481     -2   131     -7    H=   0, K=      1       4   777    795
  -2   872   -743                                                  5    46     -9
                     H=   7, K=      0       1   975  -1050       6   337   -356
H=   2, K=      0                            2  1041    933       7   251    248
                       0   982    928       3   749    706       8   293   -323
   0   295   -349      2   120     47       4   507   -527       9   603   -608
   2  2513   2456      4   225   -217       5   743   -666      10   423    429
   4   780   -742      6   684    681       6   429    393      11   197    216
   6   762   -757    -14   699   -702       7   476   -437     -14   117    115
   8   652    664    -12   111     87       8   562    554     -13   406    408
  10   411   -425    -10   316    310       9   571    584     -12   285    294
  12   -39    -46     -8   936   -901      10   -36      1     -11    82     74
 -14   154   -170     -6   215    200      11   376    385     -10   586   -587
 -12   545   -550     -4   265    278      12    91    -98      -9   317   -325
 -10   671    664     -2   626   -598      13   194   -201      -8   448    447
  -8   722   -699                                                 -7   903    859
  -6   608   -599    H=   8, K=      0    H=   1, K=      1      -6    73    -63
  -4  2891   2893                                                 -5   -33     49
  -2   353   -410      0   615   -603       0   986   -944      -4   291   -361
                       2   995   1002       1   418   -337      -3   134    -82
H=   3, K=      0      4   299   -308       2   391    454      -2    76     57
                       6   207   -194       3   189    145      -1   344    434
   0   440   -359    -14   507   -516       4   447   -432
   2   672    671    -12   102    120       5   203    -53    H=   4, K=      1
   4   634    586    -10   821    843       6   231   -215
   6   841   -873     -8   962   -969       7   559   -584       0   863    838
   8   891    894     -6    49    -20       8   629    622       1  1219   1196
  10    76     71     -4  1490   1463       9   -35    -27       2   856   -894
 -14   216    231     -2   917   -952      10    77    -42       3   356   -342
 -12  1252  -1267                          11   430    438       4   635   -623
 -10   126    113    H=   9, K=      0      12   159   -177       5   375   -362
  -8   296    292                         -13   194    208       6   284    290
  -6  1856  -1946      0   600   -585     -12   316   -302       7   551    559
  -4    77    104      2   823    810     -11   312   -293       8   526   -518
  -2   331    422      4   204    217     -10    80     92       9    74    -85
                     -14   -38      5      -9   570    552      10   -40    -39
H=   4, K=      0    -12   887   -878      -8   439    445     -14   110     95
                     -10   204    195      -7   501    459     -13   144    142
   0  1678  -1691     -8   271   -254      -6  1089  -1085     -12   117    116
   2  1640  -1587     -6   673   -654      -5   -35    -98     -11   357    358
   4  1345   1351     -4   267    287      -4   167    128     -10   285   -281
   6   505   -472     -2   405    397      -3   504    559      -9  1046  -1017
   8   549   -551                          -2   296    234      -8   457    452
  10   408    406    H=  10, K=      0      -1  1065   1193      -7   352    361
 -14   405    397                                                 -6   743    763
 -12   764   -781      0   770   -758    H=   2, K=      1      -5  1176   1163
 -10   476   -464      2   374   -384                            -4  1325  -1272
  -8  1278   1307    -14   322    309       0   643   -664      -3  1037  -1107
  -6  1416  -1351    -12   367   -363       1   523   -564      -2    59    -55
  -4  1029  -1066    -10   -37     79       2   -33    -47      -1   685   -748
  -2  3017   2858     -8   350    340       3   700   -679
                      -6  1212  -1225       4   387    388    H=   5, K=      1
H=   5, K=      0     -4   356   -382       5   746    779
                      -2   535    534       6   421   -416       0   776    804
   0   116    -67                           7   213   -206       1   -30     79
   2   942   -957    H=  11, K=      0       8   108   -101       2    46      4
   4  1210   1165                            9   128   -120       3   229    196
   L    FO     FC

   4   404   -418
   5   373   -372
   6   220    223
   7   109     95
   8    78    -78
   9   306    310
 -15   -41    -72
 -14   347   -353
 -13   333   -339
 -12   188   -182
 -11    59     74
 -10   496    503
  -9    71      6
  -8   339   -364
  -7   103   -154
  -6   168    150
  -5   506    505
  -4   469    452
  -3   266   -203
  -2   534   -534
  -1   852   -799

 H=     6,  K=    1

   0   136   -154
   1   406   -388
   2   491    470
   3   512    544
   4   345   -340
   5   108    -86
   6   280   -257
   7   204   -190
   8   262    252
 -15   276    284
 -14   227   -212
 -13   435   -427
 -12   263   -276
 -11    89    -56
 -10   312    303
  -9   615    628
  -8   520   -515
  -7   617   -615
  -6   546   -486
  -5   519   -511
  -4   929    935
  -3   845    832
  -2  1046  -1061
  -1   969   -993

 H=     7,  K=    1

   0   470   -464
   1   493   -479
   2   388    398
   3   213    193
   4   301   -292
   5   112     82
   6   275   -283
   7   374   -352
 -15   423    409
 -14   150    137
 -13    83    -59
 -12   404   -393
 -11   197   -204
 -10   245    236
  -9   603    588
  -8   425    410
  -7   226    207
  -6   440   -457
  -5   355   -327
  -4   300    280
  -3   420    435
  -2   133    -83
  -1   411   -410

 H=     8,  K=    1

   0   486   -497
   1   349   -335
   2   358   -342
```

```
   L    FO     FC

   3   226   -212
   4   419    420
   5   362    364
 -15   194    198
 -14    80     61
 -13   397    416
 -12   391   -398
 -11   816   -797
 -10   142    136
  -9   269    260
  -8   568    569
  -7   683    669
  -6   746   -721
  -5   723   -744
  -4   148   -127
  -3   422   -432
  -2   755    751
  -1   765    772

 H=     9,  K=    1

   0   225   -200
   1   118   -128
   2   386   -392
   3   502   -511
   4   325    333
 -14   288    297
 -13   563    576
 -12   336    328
 -11   146    146
 -10   241   -236
  -9   -36    -29
  -8    74     65
  -7   403    399
  -6   297    293
  -5   245   -241
  -4   347   -328
  -3   253   -250
  -2   134    142
  -1    87     96

 H=    10,  K=    1

   0   305    294
   1   336    333
   2   331   -316
 -14   -39     62
 -13    92    104
 -12   444    459
 -11   400    413
 -10   121   -102
  -9   432   -420
  -8   -37     44
  -7    67    -49
  -6   749    762
  -5   537    531
  -4   151   -150
  -3    77    -39
  -2   340   -359
  -1   -36    -20

 H=    11,  K=    1

   0   265    265
   1   267    246
 -13   220   -233
 -12   194    191
 -11   277    289
 -10   404    386
  -9   123   -121
  -8   249   -239
  -7   428   -446
  -6   364    388
  -5   220    238
  -4   114    124
  -3   297   -275
  -2   132   -140
  -1   219   -224

 H=    12,  K=    1
```

```
   L    FO     FC


 -12   131    116
 -11   204    199
 -10   450    448
  -9   471    466
  -8   479   -467
  -7   576   -582
  -6   140    132
  -5    91     75
  -4   431    449
  -3   442    460
  -2   346   -347

 H=    13,  K=    1

 -10   130    127
  -9   159    163
  -8   219    203
  -7   294   -284
  -6    67    -68
  -5   178   -174

 H=     0,  K=    2

   0   185   -243
   1  1991  -2018
   2   -32     19
   3  1009  -1062
   4   166   -145
   5  1496   1389
   6    43     40
   7   145   -126
   8   -32     43
   9   691   -657
  10   160   -152
  11   175    157
  12   123    117
  13    54    -31

 H=     1,  K=    2

   0    61    -17
   1   363   -271
   2    93     86
   3   826    865
   4    52    -52
   5   667    695
   6   239   -227
   7    90     63
   8   187    173
   9   265   -285
  10    73    -52
  11    67      7
  12   144   -100
 -13   406    416
 -12   219    224
 -11   107   -113
 -10   193   -186
  -9   248   -217
  -8   -31      8
  -7   163   -128
  -6   311    289
  -5   463    413
  -4   212   -199
  -3    79    -85
  -2    82    -70
  -1  1156   1125

 H=     2,  K=    2

   0   126     85
   1   938    866
   2   -33    -13
   3   507    440
   4    53    -49
   5   157   -181
   6    76    -63
   7   460    467
   8    73     80
   9   162    174
```

```
   L    FO     FC

  10   -36     25
  11    91    -85
 -14   172   -179
 -13    76     56
 -12   109    111
 -11   111     93
 -10   117    115
  -9   502   -527
  -8   196   -176
  -7   437    465
  -6   157    193
  -5   495   -415
  -4   -33    -43
  -3   270   -165
  -2   -33    -57
  -1   -33     51

 H=     3,  K=    2

   0    60    -37
   1   233   -103
   2   -33    -15
   3   -33     53
   4   117     95
   5   109   -114
   6   -33    -17
   7   238    228
   8   107   -107
   9   268   -260
  10    61    107
  11   196   -200
 -14   140   -134
 -13   450   -449
 -12    52    -22
 -11   484    500
 -10   314    320
  -9   172   -143
  -8   287   -301
  -7   490   -506
  -6    52     11
  -5   -32    -64
  -4   387    400
  -3   414    356
  -2   191   -142
  -1   638    623

 H=     4,  K=    2

   0    62    -81
   1   479   -549
   2   138    134
   3  1345   1276
   4   -32     64
   5    59    -22
   6    53    -16
   7   428   -403
   8   -37    -56
   9   284    282
  10    75     80
 -14    95     91
 -13   595   -608
 -12   223   -218
 -11   175    150
 -10   134    123
  -9   124   -129
  -8    77     76
  -7  1447  -1402
  -6   207   -206
  -5   227    288
  -4   307    296
  -3    72     89
  -2   -33    -70
  -1   268   -283

 H=     5,  K=    2

   0    78    -60
   1   113    130
   2    53     26
   3    47      8
```

```
    L     FO      FC

    4    -34     -76
    5    521    -539
    6    111     105
    7    417    -435
    8     61      -5
    9    238     242
  -15    473     495
  -14    214     213
  -13    374    -391
  -12    252    -251
  -11    522    -500
  -10     67     -47
   -9     83      69
   -8    338     345
   -7     54     -56
   -6    323    -318
   -5   1264   -1245
   -4     99     -90
   -3    209    -204
   -2    179     207
   -1   1066    -996

 H=     6,  K=     2

    0     62     -73
    1     89    -120
    2    134    -126
    3     71     -89
    4    -36      52
    5    310    -313
    6    -37      37
    7    -39     -65
    8    -39     -16
  -15    144     129
  -14    124     126
  -13    236    -231
  -12    121      88
  -11    166    -158
  -10    256    -250
   -9    366     382
   -8    202     200
   -7    149    -114
   -6     71     -86
   -5    399    -383
   -4    180    -188
   -3    270     257
   -2    197     201
   -1    136     125

 H=     7,  K=     2

    0    -34      63
    1    289    -264
    2     61     -29
    3    135     143
    4     65     -21
    5     79      55
    6    -38     -31
    7    129    -108
  -15    325    -323
  -14    -38     -23
  -13    170     168
  -12    284     292
  -11     59     -44
  -10    312    -319
   -9    535    -528
   -8     58      -4
   -7    -32      -7
   -6    311     315
   -5     64     -26
   -4    260    -245
   -3    137     123
   -2     94     -65
   -1     57      68

 H=     8,  K=     2

    0    163     171
    1    614     593
    2    -36     -29
```

```
    L     FO      FC

    3    105    -105
    4    136    -103
    5    280    -252
  -15    273    -276
  -14    229    -217
  -13    532     521
  -12    175     177
  -11     57      15
  -10     63      30
   -9    606    -594
   -8    180    -180
   -7    702     710
   -6    242     236
   -5    269     286
   -4     82    -101
   -3    389    -391
   -2    161    -159
   -1     72     -95

 H=     9,  K=     2

    0    -36       3
    1    375     390
    2     62       0
    3    -39      62
    4    -38     -27
  -14    196    -205
  -13    321    -317
  -12    -36      13
  -11    293     301
  -10    313     316
   -9    140    -143
   -8    240    -242
   -7     71      76
   -6    -35     -12
   -5    354     322
   -4    200     216
   -3    211     228
   -2    111    -115
   -1    -36      42

 H=    10,  K=     2

    0     86     -90
    1     89      78
    2    111     120
  -14    -39      56
  -13    349    -320
  -12    200    -202
  -11    272     284
  -10    203     201
   -9    397    -390
   -8    -36     -23
   -7    412    -402
   -6    121    -122
   -5    315     312
   -4    244     246
   -3    336     317
   -2     59     -52
   -1    217    -226

 H=    11,  K=     2

    0     67     -52
  -13     84      64
  -12    255    -253
  -11    264    -268
  -10    -37      -5
   -9     72     -54
   -8    244     256
   -7    105    -113
   -6    214    -210
   -5     65      71
   -4    -36       7
   -3    154    -123
   -2     98     101
   -1    242    -252

 H=    12,  K=     2
```

```
    L     FO      FC

  -12    -39      -6
  -11    561    -561
  -10    146    -142
   -9    195     194
   -8    184     191
   -7    320     323
   -6     83     -77
   -5    549    -555
   -4    117    -103
   -3    -39      24
   -2    159     172

 H=    13,  K=     2

   -9    275    -267
   -8    -40      -8
   -7    -40      19
   -6    150     136

 H=     0,  K=     3

    1    579     608
    2    178    -267
    3    390     354
    4    411     331
    5    114      79
    6    165     139
    7    256     254
    8    200     214
    9     96     -95
   10    257     257
   11    606    -609
   12    294    -286
   13     96      93

 H=     1,  K=     3

    0    256    -232
    1    681    -710
    2    350    -238
    3    257     276
    4     52      -1
    5    445     496
    6     90      65
    7    111     126
    8     94      53
    9    206     204
   10    183     169
   11    304    -317
   12     75     -93
  -13    114    -127
  -12     59     -10
  -11     55     -13
  -10     55     -20
   -9    293    -290
   -8    -32      64
   -7    287    -282
   -6    240    -252
   -5    693    -674
   -4    207    -239
   -3    154     145
   -2    288     213
   -1    465    -488

 H=     2,  K=     3

    0    649     621
    1    238    -211
    2     64    -145
    3    504     502
    4    138    -163
    5     67     -78
    6    100     119
    7    214    -223
    8    233    -224
    9     66      70
   10     53      53
   11    154    -153
  -14     98      88
  -13    137    -151
```

```
    L     FO      FC

  -12     97    -101
  -11    115     103
  -10    208     204
   -9    285    -293
   -8    181    -195
   -7    151    -136
   -6     93     114
   -5    615     618
   -4     87     160
   -3    398    -384
   -2    517    -467
   -1    672     698

 H=     3,  K=     3

    0     55      97
    1    541     530
    2    345    -298
    3     86      86
    4    114     133
    5    325     326
    6    -33     -17
    7     81     -77
    8    123    -137
    9    321     317
   10    111     111
  -14    -39      49
  -13    266    -259
  -12    -37      16
  -11    -35     -36
  -10    108    -114
   -9     97    -101
   -8    158     155
   -7    389    -378
   -6    350    -362
   -5    -32      13
   -4    376     308
   -3    781    -771
   -2    371    -351
   -1    269     232

 H=     4,  K=     3

    0    -33     -95
    1    460    -469
    2     52     -68
    3    237    -241
    4    608    -605
    5    303     313
    6    -34      10
    7    142    -139
    8    208    -195
    9    199    -197
   10    165    -167
  -14    246     230
  -13    220    -229
  -12    129    -123
  -11    -35      32
  -10    150    -155
   -9    694     693
   -8    503     490
   -7    638    -652
   -6     80     -46
   -5    325    -327
   -4    412    -361
   -3    352     393
   -2     53     -37
   -1    487     494

 H=     5,  K=     3

    0    106     149
    1    330     316
    2    172     176
    3    -32     -36
    4    153    -156
    5    -36     -21
    6    217    -218
    7    103      97
    8    116     108
   L    FO     FC

   9   281   -269
 -14   125   -121
 -13   163    159
 -12   239   -229
 -11   188    191
 -10   167    170
  -9   -32     34
  -8   139    114
  -7   378   -345
  -6   101   -129
  -5   132    139
  -4   179    141
  -3   319    301
  -2    71    -67
  -1    85     63

H=     6,  K=    3

   0   157   -188
   1   425    417
   2   -33    -29
   3    89    -97
   4   -35     24
   5   283   -292
   6   372   -359
   7   210    197
   8   130    131
 -14   225   -223
 -13   231    218
 -12    95    -91
 -11   -35    -35
 -10   -34      8
  -9   200   -197
  -8   152   -128
  -7   273    276
  -6   367   -333
  -5   332    330
  -4   129    143
  -3   156   -159
  -2   247   -249
  -1   432    433

H=     7,  K=    3

   0   153   -142
   1    70     38
   2   -36     -7
   3   129    130
   4   101    -95
   5    60    -44
   6   131   -138
 -14    81    -62
 -13   -36    -34
 -12   -37    -35
 -11    60     -9
 -10   124    120
  -9   191   -190
  -8   132    111
  -7   286   -265
  -6    60    -14
  -5   130   -134
  -4    64     44
  -3   -32     40
  -2   119    -83
  -1   497    485

H=     8,  K=    3

   0    62    -73
   1    56    -74
   2   316   -325
   3   288    287
   4   192    189
   5   101    -97
 -14   -38    -24
 -13   228   -237
 -12   288   -299
 -11   552    539
 -10   229    237
  -9   293   -300
```

```
   L    FO     FC

  -8   157    169
  -7   316   -313
  -6   215   -189
  -5   344    338
  -4   106    -84
  -3   446    440
  -2   280    267
  -1   382   -362

H=     9,  K=    3

   0   -37    -34
   1   118    134
   2   183   -196
   3   284    292
   4    77     62
 -14   248    258
 -13   365   -365
 -12    79     87
 -11   271   -274
 -10    60     46
  -9   227   -230
  -8   -36    -15
  -7   -36    -44
  -6   138    142
  -5   167    157
  -4   -36    -22
  -3   100   -109
  -2   101    -84
  -1   218    213

H=    10,  K=    3

   0   -38     19
   1   145   -144
   2    64    -58
 -14   115    114
 -13   -39    -73
 -12   285    293
 -11   239   -245
 -10   -36     19
  -9   190    181
  -8    65     47
  -7    84     77
  -6   329    337
  -5   350   -350
  -4   187    208
  -3   264   -295
  -2   306   -325
  -1    94    113

H=    11,  K=    3

   0   -39     35
 -13   182    185
 -12   151    160
 -11   -37    -20
 -10   169    149
  -9   -37    -27
  -8    68    -41
  -7   234    241
  -6   246    264
  -5    82     62
  -4   -37     75
  -3   217    199
  -2   -37    -14
  -1   -39      9

H=    12,  K=    3

 -11   118   -117
 -10   248    245
  -9   380   -368
  -8   253   -238
  -7   360    366
  -6   109    117
  -5    71     52
  -4   159    160
  -3   336   -344
  -2   132   -134
```

```
   L    FO     FC

H=     0,  K=    4

   0  5197  -5249
   1   318    282
   2   210   -171
   3   403    345
   4   300    290
   5   294   -330
   6   926   -930
   7    55     64
   8   196   -179
   9   309    320
  10   536    530
  11   147   -136
  12   105   -105

H=     1,  K=    4

   0   845   -907
   1   -32     53
   2   367   -402
   3   216   -166
   4   218    247
   5   -30     47
   6   757   -722
   7   143   -149
   8   284   -280
   9   258    241
  10    68     51
  11   -37    -53
  12   170   -167
 -13   233   -230
 -12   150   -166
 -11   193    188
 -10   105   -106
  -9   -34    -22
  -8   544    578
  -7   200   -206
  -6    79     80
  -5    95     81
  -4   101     95
  -3   238   -273
  -2   236   -238
  -1   -34    -52

H=     2,  K=    4

   0   311   -259
   1   293   -320
   2   829   -837
   3    77     36
   4   118     90
   5   186    191
   6   490    475
   7   221   -203
   8   169   -174
   9   -36    -43
  10   139    124
  11   142    149
 -13   215   -227
 -12   280    287
 -11   -36     53
 -10   213   -211
  -9   303    304
  -8   418    394
  -7   442   -444
  -6    56     20
  -5    78    -62
  -4  1160  -1138
  -3   370    404
  -2   371   -324
  -1   291   -291

H=     3,  K=    4

   0   368   -386
   1   -33     20
   2    90   -103
   3   -30    -11
```

```
   L    FO     FC

   4   367   -349
   5   -32      3
   6   255    270
   7    51    -59
   8   441   -441
   9   117   -107
  10   -39    -40
 -14    63    -72
 -13    83     77
 -12   818    818
 -11   290   -287
 -10   -34     13
  -9   265    261
  -8    78     88
  -7    67    -74
  -6   786    805
  -5   -33    -52
  -4   180    169
  -3   143    119
  -2   119     38
  -1   339   -316

H=     4,  K=    4

   0   663    671
   1   -30     -9
   2  1068   1050
   3   207   -213
   4   541   -561
   5   -35     18
   6    59     45
   7   -37     70
   8   454    453
   9   113   -103
 -14   201   -192
 -13   282    270
 -12   599    611
 -11   345   -361
 -10   206    190
  -9   159    152
  -8   538   -567
  -7   461    476
  -6   739    721
  -5   444   -421
  -4   390    407
  -3    58    -48
  -2  1286  -1210
  -1   313    301

H=     5,  K=    4

   0   208    205
   1   144   -147
   2   259    271
   3   -33    -13
   4   610   -590
   5    84     77
   6   -36     38
   7    90     91
   8   411    408
 -14   281   -277
 -13   283    287
 -12   -35      4
 -11    66    -39
 -10   734    745
  -9   159   -153
  -8   206   -207
  -7   313    299
  -6   432   -410
  -5   145   -180
  -4   262    263
  -3    83     65
  -2   115   -124
  -1   292    324

H=     6,  K=    4

   0   311   -328
   1   184    182
   2   114     92
   L    FO     FC       L    FO     FC       L    FO     FC       L    FO     FC

   3   -35     28      -8   294    290       7   392    403       5   152    150
   4    84   -102      -7   212   -225       8   616   -625       6   397   -407
   5   -37    -28      -6   288    279       9   139   -135       7   438   -452
   6   106   -107      -5   -37    -65      10   124   -116       8   561    559
   7   -38     22      -4   -36      5      11   140   -143       9   205    217
  10   155     89      -3   222    232     -12   307    313     -14   280   -288
 -14   -38     41      -2   323   -312     -11   163    154     -13   134    143
 -13    73     81      -1   243   -255     -10   336   -349     -12   125   -137
 -12   166    175                           -9   159   -159     -11   263   -264
 -11   302    295    H=   10, K=    4       -8   131   -139     -10   552    538
 -10   171    158                           -7   547   -529      -9   363    341
  -9   512   -514       0   403    393      -6   923    955      -8   562   -668
  -8   -33      0       1    98    -93      -5   302    332      -7   229    217
  -7    77     83       2   323    325      -4   392   -401      -6   669   -689
  -6   961   -928     -13   244    242      -3   344   -371      -5   773   -784
  -5   350    385     -12   204    208      -2   -33     43      -4  1293   1319
  -4   316    354     -11   375   -369      -1  1045  -1095      -3   489    520
  -3   301   -303     -10    69   -107                            -2   195   -172
  -2   209   -148      -9   198    186    H=    2, K=    5        -1   558    577
  -1    75    -93      -8   -36    -16
                       -7   275    279       0  1001   1015    H=    5, K=    5
H=    7, K=    4       -6   778    777       1   402    439
                       -5   259   -260       2    52     52       0   798   -812
   0   402   -398      -4   261    270       3   269    293       1   -33      1
   1   137    159      -3    62     -1       4   623   -650       2   101    101
   2   -36    -23      -2   155   -141       5   567   -590       3   255   -242
   3    94    -73      -1   121    123       6   512    525       4   438    440
   4   137   -142                             7   364    360       5   311    309
   5    65    -53    H=   11, K=    4         8   162    173       6   324   -323
   6   323   -310                             9   133   -131       7   -39    -68
 -14   466    469       0   118    124      10   327   -344       8   -40     55
 -13   279   -282     -12   150   -149      11   335   -325     -14   305    312
 -12   -37     21     -11    77    -66     -13   284   -286     -13   133    135
 -11   273    269     -10   143    154     -12   344    347     -12   130   -129
 -10   114   -107      -9    66    -46     -11   -37    -28     -11   231    244
  -9    99    -89      -8    83     64     -10   231   -231     -10   109    -98
  -8   419    410      -7   249    241      -9   359    361      -9   323   -316
  -7   144   -145      -6   -38      0      -8   361   -356      -8   278    271
  -6   100     73      -5   172   -177      -7   471   -527      -7   206    226
  -5   292    273      -4   -37    -33      -6   822    834      -6   426   -433
  -4    99    -93      -3   -38     -4      -5   327    305      -5   241   -254
  -3   305   -303      -2   207   -212      -4   215   -229      -4    63    -59
  -2    74     78      -1   189    191      -3   423    445      -3   219   -251
  -1   -34     23                           -2   917   -923      -2   385    375
                     H=   12, K=    4       -1   448   -366      -1   814    806
H=    8, K=    4
                      -11   218    225    H=    3, K=    5     H=    6, K=    5
   0   438    445     -10   505    511
   1    68    -62      -9   314   -306       0   -33     42       0    84    -91
   2   481   -488      -8   255    262       1   114   -140       1   244    244
   3   -37     21      -7   106    101       2   774    770       2   505   -522
   4   -38     -5      -6   404   -390       3   810    825       3   415   -442
   5   -40     33      -5   195    192       4   724   -723       4   485    479
 -14   392    395      -4   439    433       5   127    -96       5   164    162
 -13   358   -360      -3   122   -126       6   219    232       6   176    173
 -12   172   -175                             7   104    -97       7   102     79
 -11   107    110    H=    0, K=    5         8   440    449     -14   425    422
 -10   444   -457                             9   390    390     -13   -38     21
  -9   309    327       1   457    498      10   471   -467     -12    55    -46
  -8   566    567       2  1245  -1224     -13   -38     -5     -11   433    422
  -7   508   -505       3   594   -591     -12   -37    -22     -10   233   -242
  -6   116   -104       4   658    664     -11   226   -235      -9   462   -468
  -5   -34     19       5   759    725     -10   500    515      -8   726    767
  -4   721   -701       6   176   -150      -9   259    272      -7   -33    -24
  -3   210    217       7   -33      2      -8   670   -674      -6   -33     33
  -2   391    409       8   785   -776      -7   413   -394      -5   662    680
  -1   134   -150       9   445   -449      -6   310    298      -4   746   -783
                       10    94     88      -5   308   -309      -3   612   -595
H=    9, K=    4       11    75    -80      -4   385    375      -2  1163   1200
                       12   195    207      -3   417    395      -1   587    582
   0   212    203                           -2   209   -237
   1   101    -96    H=    1, K=    5       -1   153   -238    H=    7, K=    5
   2   410   -403
   3    82     79       0   822    819    H=    4, K=    5        0   367    370
 -14   -39     40       1   597    572                             1   506    510
 -13   -38    -23       2   444   -446       0   847   -875       2   488   -464
 -12   598    592       3   286   -268       1   715   -728       3   177   -158
 -11   159   -165       4   219    246       2   968   1006       4   319    308
 -10    69    -59       5    78    -37       3   401    391       5    88    -91
  -9   277    273       6   403    411       4   454    459       6   333    322
```

```
   L    FO    FC

 -14   154   130
 -13   135  -127
 -12   332   322
 -11   106   102
 -10   499  -480
  -9   246  -217
  -8    74     5
  -7   426  -429
  -6   329   310
  -5   415   421
  -4   437  -436
  -3   227  -230
  -2   319   316
  -1    84   -16

H=    8,  K=    5

   0   632   639
   1   250   245
   2   171   160
   3   136   137
   4   418  -412
 -14   -39   -19
 -13   282  -284
 -12   582   594
 -11   243   236
 -10   433  -432
  -9   237   225
  -8   418  -429
  -7   475  -476
  -6   867   903
  -5   238   247
  -4   195  -195
  -3   463   491
  -2   606  -617
  -1   585  -598

H=    9,  K=    5

   0   369   352
   1    94   -73
   2   356   350
   3   420   425
 -13   143  -158
 -12   -38     5
 -11   318  -312
 -10   126   110
  -9   106   104
  -8   273  -281
  -7   107   -99
  -6    77    73
  -5    82   -87
  -4   227   203
  -3   411   397
  -2   277  -268
  -1   -37    14

H=   10,  K=    5

   0   245  -249
   1   248  -261
 -13   240   235
 -12   313  -316
 -11   325  -323
 -10   304   302
  -9   -36    -9
  -8   350  -356
  -7   375   378
  -6   600  -611
  -5   349  -336
  -4   363   361
  -3    89  -104
  -2    92    91
  -1   133   127

H=   11,  K=    5

 -12   341  -350
 -11   -39   -58
 -10    84   -64
```

```
   L    FO    FC

  -9   116  -115
  -8   119   100
  -7   470   476
  -6   468  -483
  -5    83   -78
  -4   102    99
  -3   -39   -16
  -2    75    64
  -1   311   305

H=   12,  K=    5

 -10   311  -302
  -9   369  -359
  -8   559   568
  -7   215   217
  -6   354  -358
  -5    98   100
  -4   327  -338

H=    0,  K=    6

   0   584   605
   1  2129  2158
   2   -30    -9
   3   299   313
   4    56   -63
   5  1473 -1436
   6   154   154
   7   777   775
   8   -35    23
   9   236   229
  10   -36    -5
  11   356  -352
  12    83   -60

H=    1,  K=    6

   0   224   172
   1   226   196
   2   -30   -23
   3   373   355
   4    85   -59
   5  1179 -1174
   6   329   335
   7    60    70
   8    94   -62
   9   459   472
  10    67   -64
  11   318  -299
 -12   129  -138
 -11   -36   -22
 -10   186   185
  -9   612   599
  -8   195  -186
  -7   411  -428
  -6   186  -172
  -5   200  -185
  -4   191   207
  -3   846   878
  -2    74   -80
  -1  1622 -1590

H=    2,  K=    6

   0   187  -125
   1  1231 -1244
   2   243   252
   3   703   712
   4    66    52
   5   151  -171
   6   103  -110
   7   670  -685
   8   -36    39
   9   371   377
  10   -39    -6
 -13    89    77
 -12    80   -72
 -11   494  -496
 -10   -36   -19
```

```
   L    FO    FC

  -9   731   737
  -8    69   -92
  -7    64   -68
  -6    81  -101
  -5   623  -647
  -4   264   265
  -3   960   972
  -2   257  -244
  -1   108   -99

H=    3,  K=    6

   0    54   -93
   1   841  -860
   2   123   133
   3    81    65
   4    79   -65
   5   570   585
   6    99  -102
   7   615  -621
   8   161   169
   9   358   350
 -13   549   551
 -12   136  -128
 -11   597  -598
 -10   204  -197
  -9    80    75
  -8   249   281
  -7   860   875
  -6   221  -217
  -5   745  -746
  -4   247  -257
  -3    45   -37
  -2   119    99
  -1   483   475

H=    4,  K=    6

   0   133  -125
   1    53    67
   2   255  -264
   3  1300 -1310
   4    90    80
   5   694   692
   6   -36   -22
   7    95    78
   8   -40   -30
   9   386  -403
 -13   625   637
 -12   -39    23
 -11   -36    21
 -10   -36    13
  -9   465  -473
  -8   -34    42
  -7  1394  1418
  -6   100  -101
  -5    69   -83
  -4   271  -247
  -3   896  -917
  -2   247   283
  -1  1093  1117

H=    5,  K=    6

   0   -33    18
   1   524   517
   2   145  -150
   3   620  -643
   4   182   202
   5   544   542
   6   121  -118
   7   562   574
   8    88  -103
 -13   283   277
 -12   218   218
 -11   650   658
 -10    65   -50
  -9   463  -468
  -8   167  -164
  -7   120   122
```

```
   L    FO    FC

  -6   251   260
  -5  1315  1344
  -4   -32    -1
  -3   697  -686
  -2   -32   -43
  -1   711   692

H=    6,  K=    6

   0   263   258
   1   670   715
   2    64    59
   3   204  -204
   4    89  -108
   5   -37   -19
   6   -39    51
 -13   -38   -43
 -12   -36   -12
 -11   382   382
 -10   -36    23
  -9   162  -156
  -8    52   -58
  -7   456  -477
  -6   281   268
  -5   871   892
  -4   -34   -41
  -3   248  -257
  -2   160  -148
  -1   574  -580

H=    7,  K=    6

   0    80    73
   1   325   300
   2   -38     4
   3   211   212
   4    63   -24
   5   401  -384
 -13   264  -247
 -12   159  -157
 -11    76    75
 -10   264   270
  -9   676   681
  -8   100   -98
  -7   488  -475
  -6   154  -147
  -5   139   128
  -4   175   164
  -3   416   424
  -2   -36    45
  -1   633  -649

H=    8,  K=    6

   0   181  -176
   1   662  -673
   2   144   136
   3   496   504
   4    91    92
 -13   346  -344
 -12    65   -59
 -11   257  -273
 -10    53    46
  -9   741   738
  -8    76   -70
  -7   469  -475
  -6   138  -128
  -5   582  -576
  -4   239   242
  -3   758   778
  -2   -37    25
  -1   138  -133

H=    9,  K=    6

   0   -39   -42
   1   646  -654
   2   119   128
 -13   333   326
 -12    71   -94
```

```
   L    FO    FC       L    FO    FC       L    FO    FC       L    FO    FC

 -11   438  -447      -4   355  -331                            -8    93   -98
 -10   219  -214      -3    75    84    H=    5, K=    7      -7   398   410
  -9   209   199      -2    95   -84                            -6   255   259
  -8   101   105      -1   573   568       0   271  -291      -5   215  -219
  -7   216   222                           1   -35     0      -4   221  -223
  -6   -37   -13    H=    2, K=    7       2    55   -67      -3   465  -456
  -5   660  -653                           3   102    96      -2   152  -139
  -4    99   -76       0   -30   -23       4   279   276      -1   464   455
  -3    64   -58       1   104   -89       5   206  -202
  -2   -37    13       2    64   -36       6    84    81    H=    9, K=    7
  -1   313   304       3   425  -427       7    76    87
                       4   170  -163     -13   166  -152       0   126   118
H=   10, K=    6       5   293   298     -12    81   -91       1   -39    -7
                       6   164   159     -11   267  -269       2   166   164
   0   -39   -11       7   -36   -43     -10   233   222     -12   267   263
 -12   -40    35       8   121   121      -9   260   257     -11   405   400
 -11   205  -199       9   -37   -15      -8    51   -36     -10   123  -123
 -10    82   -81      10   213  -201      -7    51   -26      -9   -37    31
  -9    85    60     -12   328   332      -6   314  -310      -8   293  -288
  -8    68    75     -11   -37    36      -5    74   -79      -7   -36     7
  -7   569   566     -10   250  -249      -4   263   271      -6   231   222
  -6    76   -79      -9   -35   -48      -3   141   126      -5   113   116
  -5   351  -353      -8   -35   -43      -2   233   244      -4   -36   -12
  -4   235  -229      -7   360   368      -1   437  -447      -3   166  -170
  -3   401  -415      -6   258   256                            -2   188  -193
  -2   132   122      -5   390  -391    H=    6, K=    7      -1    74   -57
  -1   514   523      -4   206  -225
                      -3   126  -132       0   134  -120    H=   10, K=    7
H=   11, K=    6      -2   -30     0       1   408  -405
                      -1   145   115       2   -35    16     -11   259   256
 -11   289   281                           3   278   290     -10   178   174
 -10   -39    -6    H=    3, K=    7       4   227   236      -9   -38   -38
  -9   200  -202                           5    55    60      -8   228  -236
  -8   180  -177       0   -31     8       6   182   175      -7   256  -251
  -7   183   178       1    85   -69     -13   -39   -17      -6   109  -117
  -6   132   125       2   406   405     -12   132  -136      -5   427   432
  -5   122   138       3   424  -434     -11   211  -211      -4   -38   -23
  -4   -38   -25       4   253  -256     -10   105  -102      -3   179   185
  -3   240  -239       5   -35     6      -9   296   302      -2   -37   -12
  -2   -39    -4       6   115  -102      -8   330   328      -1   186  -187
                       7   -36    18      -7   104  -113
H=   12, K=    6       8   264   271      -6   -35   -24    H=   11, K=    7
                       9   344  -338      -5   451  -459
  -7   347  -360     -12   239   238      -4    55   -63      -9   208   202
                     -11   259   261      -3   371   385      -8   -39   -34
H=    0, K=    7     -10    86    90      -2   376   381      -7   340  -349
                      -9   134  -126      -1   392  -398      -6   401  -419
   1   591  -572      -8   420  -425                            -5   -39   -29
   2   165  -145      -7   201   209    H=    7, K=    7      -4   197   186
   3   220   222      -6   525   527                            -3   -39    12
   4    83   102      -5   389   383       0   197   188
   5   332  -340      -4   -32    27       1   293  -302    H=    0, K=    8
   6    57   -34      -3    46   -52       2   171  -161
   7   121  -137      -2   241  -246       3    60    51       0  1791  1825
   8   350  -352      -1   -31    22       4   108   112       1   173  -163
   9   216   235                           5    90    53       2   342   336
  10   -36     3    H=    4, K=    7     -13   207   222       3   164  -138
  11   292   285                         -12    85   -84       4   -33   -43
                       0   -32    -9     -11   108  -100       5   -33    44
H=    1, K=    7       1   591   588     -10   363  -370       6   266   260
                       2   262   291      -9    93    56       7    71   -65
   0   517   496       3   -35   -33      -8   310   307       8   277   252
   1   192  -213       4   193   206      -7   466   468       9    73   -74
   2   155  -179       5   237  -247      -6    57     8      10   372  -355
   3   148   143       6   135  -131      -5   194  -199
   4   180  -189       7   246   250      -4   388  -389    H=    1, K=    8
   5   249  -256       8   313   311      -3    77    58
   6   249   251     -13   -40    -4      -2   289   272       0   396   392
   7   325  -333     -12   -37    11      -1   175  -147       1   -31   -56
   8   104   -97     -11   -37    74                             2   127   128
   9    92    74     -10   429   438    H=    8, K=    7       3   272   271
  10   238  -232      -9   341  -351                             4   -33    64
 -12    64    60      -8   433  -431       0   245   262       5   -34   -23
 -11    77   -64      -7   120   110       1   -39   -47       6   169   160
 -10   252  -266      -6    49   -36       2   -38     0       7    94   -83
  -9   106   114      -5   491   507       3   281  -270       8   197   206
  -8   220   216      -4   509   516     -12   416   417       9   -36   -26
  -7   493   503      -3   278  -265     -11   246  -244      10    99   102
  -6   228   230      -2   177  -190     -10   393  -395     -11   110   108
  -5    63   -39      -1   516  -515      -9   -36   -28     -10   110  -116
```

```
   L    FO     FC

  -9   -36    -21
  -8   133   -124
  -7   -35    -39
  -6    53     -1
  -5   192    205
  -4   232   -235
  -3   155    187
  -2   270    282
  -1   -32    -33

H=    2, K=     8

   0   350    359
   1   182    195
   2    89     63
   3   -33     21
   4   133    125
   5   -36    -52
   6   268   -245
   7   -35     14
   8   -36    -26
   9    74     76
 -11   -38    -22
 -10   -35     17
  -9   -35     16
  -8   223   -207
  -7    88     68
  -6   209    211
  -5   115    107
  -4   205    194
  -3   114   -129
  -2   389    379
  -1   107    130

H=    3, K=     8

   0   323    340
   1    56    -82
   2    91    -89
   3   -35      0
   4   204    218
   5    92    102
   6   -36     10
   7    54     38
   8    93    100
 -12   437   -422
 -11   -37     -5
 -10   -36     43
  -9   141    132
  -8   281   -283
  -7    67    -50
  -6   213   -213
  -5   169   -163
  -4   -33    -18
  -3   193    205
  -2   141   -134
  -1   207    194

H=    4, K=     8

   0    94   -120
   1    95    -76
   2   460   -458
   3   147    145
   4   125    132
   5   -36     37
   6   111    121
   7   -39      6
 -12   459   -461
 -11   -36    -20
 -10    61    -36
  -9    68    -57
  -8   129    146
  -7   137   -129
  -6   282   -286
  -5   -33    -11
  -4   -33     32
  -3   132    126
  -2   247    234
  -1    82    -96
```

```
   L    FO     FC

H=    5, K=     8

   0   147   -150
   1    81     71
   2   -36     16
   3   -36    -42
   4   195    194
   5    96   -101
   6    63     42
 -12   204   -204
 -11   -37    -61
 -10   373   -365
  -9   154   -144
  -8   148    156
  -7   140    143
  -6   -35     46
  -5   -34    -21
  -4    84    -71
  -3   234   -222
  -2    69     48
  -1   -35    -47

H=    6, K=     8

   0   136   -117
   1    80    -57
   2    97     88
   3    90    -97
   4   109    123
   5   -38    -23
 -12   198   -193
 -11   -37      7
 -10   119   -120
  -9   -36     36
  -8   139    139
  -7   106     95
  -6   272    257
  -5   101    -94
  -4    53    -66
  -3   -35    -43
  -2   190    184
  -1   148    159

H=    7, K=     8

   0    90     96
   1   -36     20
   2    59     50
   3    86     63
   4   236    232
 -12    57     26
 -11   162    159
 -10   115   -108
  -9    96    -93
  -8   148   -150
  -7   100    -89
  -6   -35    -19
  -5   132    135
  -4   -36    -39
  -3   131    112
  -2   -36     35
  -1   123   -137

H=    8, K=     8

   0   209   -205
   1   120    122
   2   119    133
 -12   194    184
 -11    66     54
 -10   193    206
  -9   -37    -59
  -8   284   -289
  -7    72     61
  -6   168    162
  -5   148    151
  -4   153    139
  -3   -35    -26
  -2   110   -118
```

```
   L    FO     FC

  -1    75    -84

H=    9, K=     8

   0   -39    -34
 -11    89    -90
 -10   120    111
  -9   131    137
  -8   292   -286
  -7   -37     30
  -6   116   -115
  -5    87    -82
  -4   -37    -34
  -3   -39     65
  -2   187    192
  -1   134    132

H=   10, K=     8

 -10   126    133
  -9   -38     -1
  -8   132   -137
  -7   105    -88
  -6   414   -408
  -5    87    -89
  -4    71    -81
  -3   147    151
  -2    87    -78

H=    0, K=     9

   1    74     72
   2   194    191
   3    88    -86
   4    88     76
   5   169   -158
   6   -35     30
   7   147    131
   8   287    278
   9    80     81
  10   168    171

H=    1, K=     9

   0    59    -26
   1   -34    -21
   2   201   -214
   3   -34    -37
   4   -34     26
   5   -36     25
   6   -35     -3
   7   -36     21
   8   -38     62
   9    66    -53
 -10    91     85
  -9    52     25
  -8    84    -70
  -7    92    100
  -6   143   -142
  -5   -34     27
  -4   110    -93
  -3    93     84
  -2    57    -53
  -1   444    453

H=    2, K=     9

   0   -34    -29
   1   -33     35
   2    96   -102
   3   -35      6
   4    73     80
   5   -36     33
   6   -36     41
   7   -37    -44
   8   196   -200
 -11   -40     47
 -10   220    209
  -9   109    -91
  -8    72    -69
```

```
   L    FO     FC

  -7   -35    -33
  -6   210   -210
  -5   -35     46
  -4   144    133
  -3   -33    -34
  -2   -34     45
  -1   210   -217

H=    3, K=     9

   0    69     47
   1   -34     43
   2    99   -109
   3   221   -228
   4   -35     -8
   5   117   -126
   6   -36     37
   7    73     44
   8   156   -142
 -11   -37      2
 -10    69    -58
  -9   -36      8
  -8   181    174
  -7   131    127
  -6   250   -254
  -5   -33      7
  -4   129    148
  -3   -34      9
  -2   273   -269
  -1    63    -57

H=    4, K=     9

   0   128    123
   1    58    -49
   2   140   -152
   3   -36    -32
   4   351   -351
   5   -37    -22
   6    62     50
   7   118    105
 -11   -38      7
 -10   193   -188
  -9    57    -69
  -8   408    409
  -7    55    -38
  -6   -36     30
  -5    58     50
  -4   308   -302
  -3   -34    -43
  -2   -34     11
  -1   128   -134

H=    5, K=     9

   0    78     59
   1   221   -225
   2    74     60
   3   132    129
   4    96    -98
   5   -37     13
   6    99    -90
 -11   221   -216
 -10   -36    -24
  -9    99     97
  -8   109    122
  -7    73     71
  -6   -35    -39
  -5    75     46
  -4   -35     -3
  -3    91     94
  -2    70     72
  -1   228   -220

H=    6, K=     9

   0   -36    -28
   1    57    -33
   2    66     77
   3   -37     43
   L     FO     FC

   4     58    -44
 -11    233   -231
 -10    -37    -10
  -9     73     72
  -8    236   -231
  -7    245    243
  -6    -36    -35
  -5    252   -264
  -4    117    123
  -3    -36     -4
  -2    333   -324
  -1     71    -82

H=     7,  K=    9

   0    -36    -27
   1    143   -137
   2     56    -20
   3    -40    -51
 -11     90     79
 -10    192    182
  -9     91     64
  -8     63    -43
  -7    165    162
  -6    -36     39
  -5    -36    -72
  -4    -35    -15
  -3    -36     -8
  -2    127   -142
  -1    -36     28

H=     8,  K=    9

   0    123   -130
   1    -38      8
 -10    269    271
  -9    126   -128
  -8     94     96
  -7    -37     33
  -6    265   -277
  -5     80     64
  -4    -37     71
  -3    214   -213
  -2    152    147
  -1    124    120

H=     9,  K=    9

  -9     58     31
  -8     72     50
  -7     61    -53
  -6    -38    -32
  -5    -38     17
  -4    -38     32
  -3    159   -139
  -2     79    -61
  -1    165   -155

H=    10,  K=    9

  -7    244   -247
  -6    263    262
  -5    -39    -30
  -4    -38    -15

H=     0,  K=   10

   0    376   -386
   1    859   -854
   2     56    -55
   3     79    -68
   4    154    149
   5    572    558
   6    164   -165
   7    343   -333
   8    121   -117
   9     65    -59

H=     1,  K=   10
```

```
   L     FO     FC

   0    144   -133
   1     64    -74
   2    -35    -30
   3    167   -145
   4    -36     30
   5    513    505
   6    110   -107
   7    -38     -9
   8    139   -136
  -9    247   -249
  -8    193    185
  -7    112    121
  -6    104    -88
  -5    -35     16
  -4    -35     29
  -3    316   -311
  -2    -35     43
  -1    621    619

H=     2,  K=   10

   0    -34      6
   1    401    405
   2    185   -180
   3    285   -288
   4     68    -64
   5    131    116
   6    185    189
   7    281    280
 -10     90    -81
  -9    300   -290
  -8    302    305
  -7     77    -71
  -6     90    -95
  -5    263    255
  -4    200   -198
  -3    288   -284
  -2    269    271
  -1    -35     16

H=     3,  K=   10

   0    -35     33
   1    335    339
   2     78    -78
   3    -37     36
   4    -37    -25
   5    277   -272
   6     98     97
   7    228    224
 -10    140   -126
  -9    -38    -52
  -8    -37     42
  -7    366   -366
  -6    176    174
  -5    301    304
  -4    -36    -28
  -3    -35      3
  -2     68     73
  -1    189   -178

H=     4,  K=   10

   0    177    179
   1    -36    -24
   2    142    139
   3    548    561
   4     98    -97
   5    360   -344
   6    -39     15
 -10    202   -196
  -9    261    256
  -8     92    -93
  -7    544   -544
  -6    319    314
  -5     95    -61
  -4    -35    -14
  -3    367    362
  -2    176   -180
  -1    413   -416
```

```
   L     FO     FC

H=     5,  K=   10

   0     90     72
   1    244   -239
   2    100     93
   3    259    266
   4    139   -133
 -10    104     88
  -9    181    197
  -8    168   -174
  -7     74    -68
  -6     92     81
  -5    606   -613
  -4    -36     -4
  -3    311    314
  -2    126   -111
  -1    225   -235

H=     6,  K=   10

   0    171   -171
   1    257   -251
   2    -38     24
   3    121    117
 -10    282    281
  -9     63    -41
  -8    183   -180
  -7    224    217
  -6    221   -202
  -5    339   -339
  -4    226    229
  -3     58     47
  -2     78    -75
  -1    195    197

H=     7,  K=   10

   0    134   -126
   1     81    -61
   2    -39     35
 -10     81     65
  -9    340   -337
  -8    114    101
  -7    211    200
  -6    163   -156
  -5     69    -22
  -4    110    108
  -3    249   -246
  -2     77    -62
  -1    287    287

H=     8,  K=   10

   0    -39     -1
  -9    304   -316
  -8    318    318
  -7    124    122
  -6    142   -144
  -5    268    258
  -4    162   -146
  -3    298   -293
  -2    122    124
  -1     63     27

H=     9,  K=   10

  -7    122   -119
  -6    -39      3
  -5    339    321
  -4    126   -114
  -3    138    129

H=     0,  K=   11

   1    407    401
   2    127    137
   3    447   -438
   4    228   -219
   5    356    345
```

```
   L     FO     FC

   6    188    178
   7    159    167
   8    145    141

H=     1,  K=   11

   0    399   -407
   1    501    495
   2    258    253
   3    249   -240
   4     71     51
   5    -39    -35
   6    169   -157
   7    420    409
  -8    -40      0
  -7    360   -366
  -6    234   -246
  -5    389    390
  -4    274    265
  -3    276   -278
  -2    113    134
  -1    430   -442

H=     2,  K=   11

   0    122   -106
   1    283    267
   2    108     88
   3    305    315
   4    145    154
   5    409   -411
   6    232   -219
  -9    120    129
  -8    182    163
  -7    464   -470
  -6    139   -152
  -5    337    349
  -4    -37    -17
  -3    235    232
  -2    168    174
  -1    420   -420

H=     3,  K=   11

   0    -37     14
   1    118   -120
   2    314   -304
   3    563    554
   4    238    247
   5    131   -136
  -9    298    284
  -8    191    198
  -7    316   -312
  -6    136   -137
  -5    286   -287
  -4    198   -205
  -3    402    390
  -2    239    239
  -1    227   -216

H=     4,  K=   11

   0     99    106
   1    525   -534
   2    246   -247
   3    233    237
   4    -40      2
  -9    305    317
  -8    -38      4
  -7    -38     39
  -6    178    170
  -5    516   -520
  -4    292   -308
  -3    327    325
  -2     51     21
  -1    334    347

H=     5,  K=   11

   0    204    197
```

L	FO	FC
1	195	-186
2	-39	34
3	112	-113
-9	170	-170
-8	132	-139
-7	253	229
-6	188	171
-5	210	-200
-4	72	-70
-3	164	-152
-2	306	-309
-1	563	559
H=	6, K=	11
0	-39	56
1	222	230
2	-40	35
-9	354	-356
-8	131	-130
-7	182	188
-6	161	-151
-5	269	272
-4	166	171
-3	432	-440
-2	247	-251
-1	418	420
H=	7, K=	11
0	204	-205
-8	62	-21
-7	267	-266
-6	136	-153
-5	341	329
-4	264	252
-3	269	-248
-2	104	-79
-1	80	38
H=	8, K=	11
-6	84	-95
-5	267	274
-4	67	34
-3	222	212
H=	0, K=	12

L	FO	FC
0	1118	-1138
1	201	189
2	75	60
3	-37	34
4	151	156
5	72	-63
6	413	-428
H=	1, K=	12
0	451	-451
1	-37	37
2	248	-235
3	-37	-19
4	360	342
5	137	-106
6	257	-247
-7	58	-40
-6	168	-161
-5	160	-155
-4	104	-102
-3	74	57
-2	327	299
-1	148	-159
H=	2, K=	12
0	55	-35
1	178	-183
2	378	-394
3	83	93
4	193	193
5	-39	-10
-7	-39	28
-6	89	82
-5	187	-182
-4	422	-436
-3	118	131
-2	-36	-11
-1	-38	-64
H=	3, K=	12
0	274	255
1	104	-102
2	199	-199
3	-38	10

L	FO	FC
4	226	-216
-7	132	136
-6	419	406
-5	-38	-13
-4	264	-249
-3	160	-155
-2	122	-114
-1	-37	44
H=	4, K=	12
0	264	268
1	-38	26
2	257	270
3	163	-155
-7	93	90
-6	241	247
-5	77	75
-4	90	90
-3	186	-189
-2	414	-422
-1	119	118
H=	5, K=	12
0	60	-28
1	71	81
-7	139	-137
-6	118	-123
-5	134	134
-4	416	420
-3	-38	7
-2	297	-277
-1	-40	-3
H=	6, K=	12
-6	346	-355
-5	67	84
-4	204	219
-3	68	60
-2	-40	-1
-1	168	-177
H=	0, K=	13
1	74	-61
2	78	-69

L	FO	FC
3	-37	12
4	-38	-16
H=	1, K=	13
0	67	81
1	-38	32
2	-37	40
3	-38	33
4	-38	-22
-5	87	45
-4	-37	-1
-3	130	-128
-2	-37	-4
-1	215	-223
H=	2, K=	13
0	-36	1
1	-37	-5
2	-37	27
3	-38	20
-5	84	90
-4	-38	-7
-3	-38	-63
-2	-37	-41
-1	93	62
H=	3, K=	13
0	62	-45
1	-38	-21
2	118	106
-5	117	101
-4	-38	26
-3	-38	18
-2	66	77
-1	67	-43
H=	4, K=	13
0	81	-83
-5	-37	-42
-4	124	119
-3	128	140
-2	59	57

FIGURE 6

THE $[Fe(DAPSC)Cl_2]^+$ COMPLEX ION

The atomic numbering scheme and 50% probability thermal ellipsoids are shown. Hydrogen atoms are omitted for clarity.

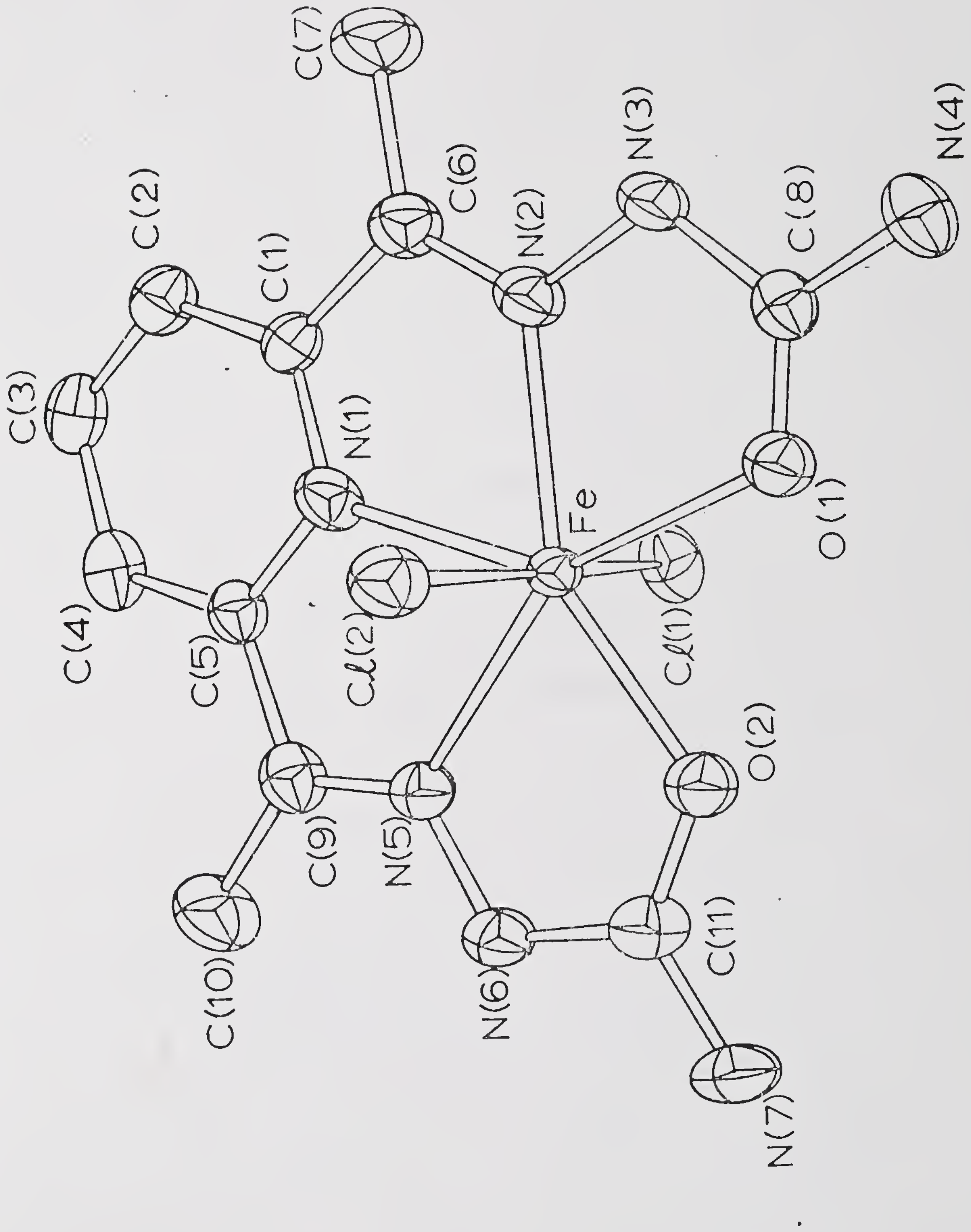
C(7)
C(6)
N(3)
N(4)
C(2)
C(1)
N(2)
C(8)
C(3)
N(1)
Fe
O(1)
C(4)
C(5)
Cℓ(2)
Cℓ(1)
O(2)
C(9)
N(5)
C(10)
N(6)
C(11)
N(7)

FIGURE 7

A PACKING DIAGRAM FOR $[Fe(DAPSC)Cl_2]Cl \cdot 2H_2O$

The view is a projection along the b axis. The atomic numbering scheme is shown. C10 and hydrogen atoms are omitted for clarity. Larger circles represent ionic chlorides. Dotted lines represent hydrogen bonds listed in Table 14. Primed and doubly primed atoms are in positions equivalent to the unprimed atoms.

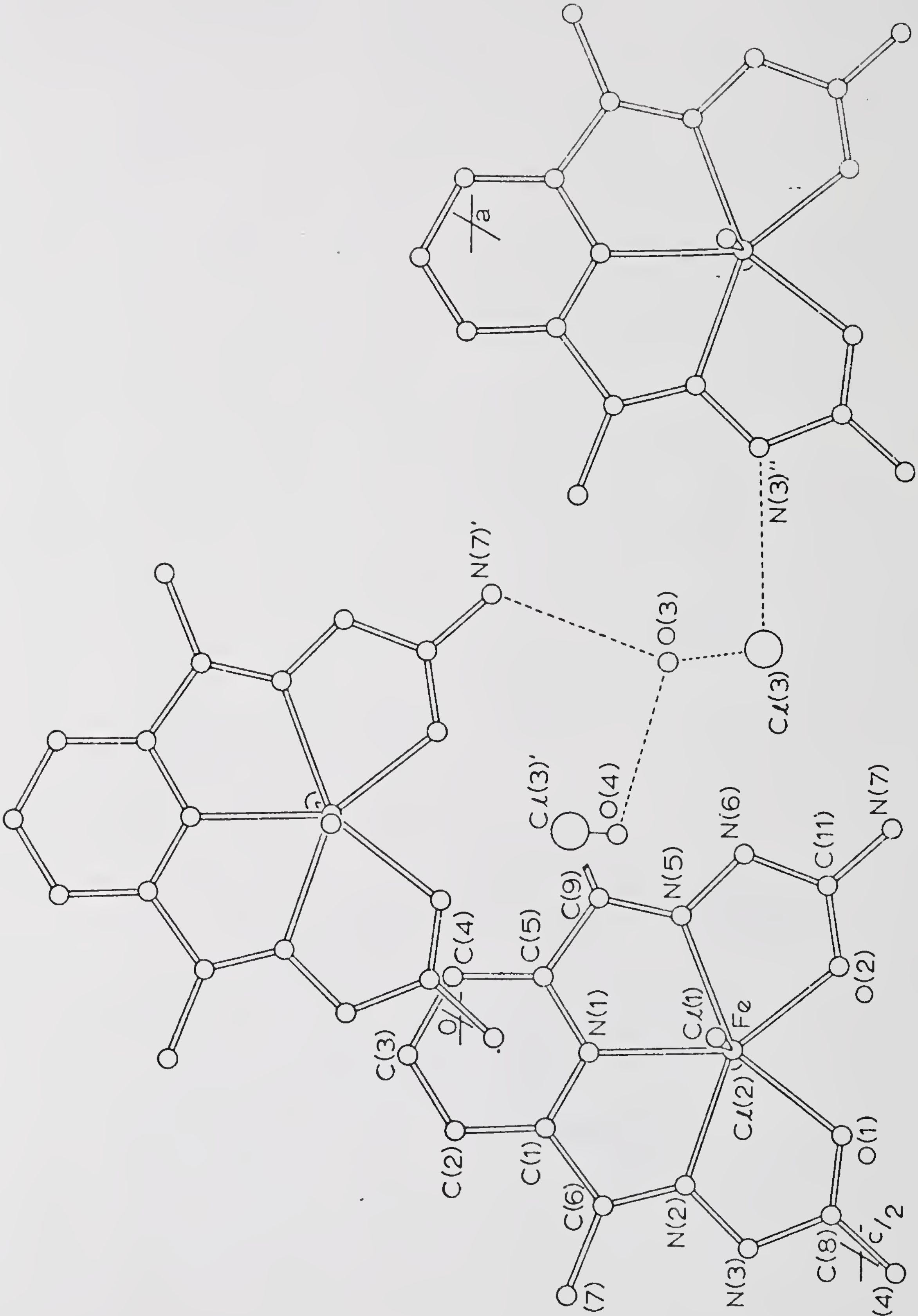
N(7)'
O(3)
Cℓ(3)
N(3)''
a
Cℓ(3)'
O(4)
N(6)
N(7)
C(11)
N(5)
C(9)
C(5)
C(4)
O(2)
N(1)
Cℓ(1)
Fe
0
C(3)
Cℓ(2)
O(1)
C(2)
C(1)
C(6)
N(2)
C(8)
c/2
N(3)
C(7)
N(4)

Table 17
AVERAGE BOND LENGTHS AND NON-BONDED CONTACTS FOR $[Fe(DAPSC)Cl_2]^+$

The distances (Å) between the atoms listed on the left are followed by their respective estimated standard deviations in parentheses. The designation (e) refers to equatorial donors.

Fe-Cl	2.34(2)
Fe-O	2.10(3)
Fe-N	2.200(2)
Cℓ...O(e)	3.22(3)
Cℓ...N(e)	3.16(3)
O(e)...O(e)	2.593(6)

is shown in Figure 7.

Discussion

The pentagonal bipyramidal geometry of the complex cation is easily seen in Figure 6. Atoms N1, N2, N5, O1 and O2 form an approximately planar pentagon around the central iron with Cℓ1 and Cℓ2 occupying the apices.

The Fe-N bond lengths are similar to those reported for two other pentagonal bipyramidal complexes of Fe(II).[4] The Fe-Cℓ bond lengths of 2.362(2) and 2.325(2) are within the range of Fe(III)-Cℓ distances previously determined.[65,80-82] The Fe-O distances of 2.131(4) and 2.074(4)Å are significantly longer than the Fe-O bond lengths in salicylaldehyde derivatives,[65] and similar to Fe-O distances found in the $Fe(H_2O)(EDTA)^-$ ion.[3]

The effect of the comparatively small (0.645Å),[83] highly charged (+3) iron ion on the bond lengths and nonbonded contacts is particularly striking. Table 17 will be referred to in the ensuing discussion. The Fe-Cℓ distance of 2.34(2)Å and the Fe-O distance of 2.10(3)Å are approximately 0.17Å and 0.09Å shorter than the respective bond lengths in $[Fe(DAPSC)(H_2O)Cl]^+$. This effect may be explained by the smaller ionic radius of iron in both cases. Additionally, the increased coulombic attraction between Fe^{+3} and $C\ell^-$ with respect to Fe^{+2} and $C\ell^-$ may account for the larger decrease in the Fe-Cℓ bond lengths. The Fe-N distance of 2.200(2)Å is remarkably similar to the Fe-N distance of 2.21(1)Å for the Fe(II) complex. Apparently the portion of the ligand containing the three nitrogen donors is fairly rigid and does not appreciably change dimensions under the influence of the more highly charged central metal ion. The decreased Fe-Cℓ bond lengths also give rise to shorter non-bonded contacts for the Fe(III) complex. The Cℓ-O contacts decrease from 3.38(1)Å to 3.22(3)Å and the Cℓ-N distances decrease from 3.35(8)Å to 3.16(3)Å. The oxygen-oxygen contact between O1 and O2 also decreases from 2.761(8)Å for Fe(II) to 2.593(6)Å for Fe(III). These decreases may all be an effect of the shorter bond distances required by the smaller, more highly charged Fe(III) ion and the shorter lengths resulting from the greater attraction between Fe(III) and $C\ell^-$ when compared to Fe(II).

The DAPSC ligand assumes a nearly planar conformation in this complex. The deviations from planarity of the five donor atoms range from only 0.025Å for N2 to 0.004Å for O2. These distortions are the smallest observed for any of the DAPSC complexes involving apical chloride ions. The fact that the DAPSC complexes with two apical water molecules also contain nearly planar DAPSC ligand vide infra suggests that the distortion of the $[M(DAPSC)(H_2O)Cl]^+$ complexes may be due to the presence of apical donors of unequal strength. The arrangement of the five planar donors is staggered. O2 is nearly on the plane, N2 and N5 are below, and N1 and O2 are above. The deviations are much less than in the case of the isomorphous M(II) complexes and for all practical purposes the donors may be called co-planar.

The bond distances and angles in the DAPSC ligand are not significantly different from those in the M(II) complexes. The conformation of the ligand is similar to the helical form observed for the M(II) complexes with the exception that O2, which would be below the plane of the pyridine ring in the helical form is actually above the plane of the pyridine ring. The dihedral angle of 2.23° between planes of the pyridine ring and the donor set is considerably less than the 5-6° angle for the M(II) complexes, and is another indication of the high degree of planarity associated with DAPSC in this complex.

The packing diagram, Figure 7, illustrates the hydrogen bonding scheme of the unit cell. The ionic chloride, Cℓ3, is hydrogen bonded to two lattice water atoms, O3 and O4, and an NH group of the semicarbazone residue, N3-H1. Lattice water, O3, is also hydrogen bonded to O4 and the NH_2 group of the semicarbazone containing N7. All distances between the hydrogen bonded atoms are greater than or equal to the sum of van der Waals radii[74] and within the limit below which hydrogen bonds are said to exist.[75] Two other hydrogen bonds may be present in the crystal structure. O1 and O2 are within hydrogen bonding distance to O4. However, the facts that O4 is hydrogen bonded to Cℓ3 and that no peak attributable to a hydrogen atom between either O1 and O4 or O2 and O4 could be found in the difference Fourier synthesis suggest that these atoms may not actually be hydrogen bonded.

Structure Solution and Refinement for $Cu(H_2O)(ASCACHOPY)Cl \cdot \frac{1}{2}H_2O$

The copper atom position was calculated from a sharpened three-dimensional Patterson function. A Fourier synthesis phased on this atom established the positions of the two chlorine atoms. Subsequent Fourier syntheses produced the positions of all non-hydrogen atoms. Three least-squares cycles with isotropic thermal parameters refined the structure, R=0.085. Three cycles of least-squares refinement with individual anisotropic thermal parameters reduced R to 0.049. The positions of all thirteen hydrogen atoms were located from a difference Fourier synthesis using the refined anisotropic atomic coordinates. The hydrogen atoms were arbitrarily assigned isotropic thermal parameters one unit greater than the refined isotropic thermal parameter of the bonded atoms. All parameter shifts were less than one-tenth of their estimated standard deviations after three additional least-squares cycles holding the hydrogens constant, R=0.039. At this point, refinement was terminated.

Results for $Cu(H_2O)(ASCACHOPY)Cl \cdot \frac{1}{2}H_2O$

The final positional and thermal parameters for the non-hydrogen atoms are listed in Table 18. The probable positional parameters and bond distances for the hydrogen atoms appear in Table 19. Intramolecular bond distances and angles, and short intermolecular contacts are given in Table 20. Least-squares planes and deviations are tabulated

Table 18

FINAL POSITIONAL AND THERMAL PARAMETERS (x 10^4) FOR THE NON-HYDROGEN ATOMS OF $Cu(H_2O)(ASCACHOPY)Cl \cdot \frac{1}{2}H_2O$ WITH THEIR RESPECTIVE ESTIMATED STANDARD DEVIATIONS IN PARENTHESES

ATOM	X	Y	Z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Cu	1756(1)	5275(1)	4317(1)	23(1)	39(1)	15(1)	8(1)	2(1)	1(1)
Cℓ	2202(1)	4158(1)	3178(1)	35(1)	51(1)	15(1)	34(1)	3(1)	-5(1)
O1	2082(2)	4034(3)	5173(2)	30(1)	42(3)	19(1)	12(3)	1(2)	-4(3)
O2	403(2)	4566(3)	4242(2)	28(1)	64(3)	47(2)	-3(3)	-1(2)	-2(4)
O3	1530(2)	6621(3)	3584(2)	46(2)	48(3)	19(1)	24(3)	7(2)	3(3)
O4	575(2)	12074(3)	3978(2)	41(2)	49(3)	47(2)	17(3)	-6(3)	18(4)
N1	1642(2)	6248(3)	5398(2)	16(1)	38(3)	18(2)	5(3)	-7(2)	8(3)
N2	1123(2)	9289(3)	4914(2)	13(1)	39(3)	27(2)	-1(3)	-1(2)	2(4)
N3	1779(2)	5528(3)	6140(2)	30(2)	39(3)	22(2)	9(3)	-8(3)	9(4)
N4	2187(2)	3669(3)	6636(2)	44(2)	48(3)	22(2)	18(4)	-14(3)	14(4)
C1	1301(2)	8134(4)	4729(3)	10(1)	41(4)	22(2)	-4(4)	2(3)	5(4)
C2	1325(2)	7709(4)	3832(3)	16(2)	44(4)	25(2)	4(4)	5(3)	6(5)
C3	1126(3)	8556(4)	3171(3)	26(2)	55(4)	25(2)	7(4)	8(3)	20(5)
C4	945(3)	9729(4)	3381(3)	22(2)	55(4)	28(2)	3(5)	7(3)	13(5)
C5	954(2)	10071(4)	4272(3)	13(2)	41(4)	28(2)	-1(4)	2(3)	7(5)
C6	780(2)	11333(4)	4539(3)	14(2)	43(4)	41(3)	-1(4)	-1(3)	16(5)
C7	862(3)	11662(4)	5490(3)	24(2)	53(4)	37(2)	-4(5)	-8(3)	-14(5)
C8	1451(2)	7367(4)	5513(2)	13(1)	45(4)	20(2)	-3(4)	-6(3)	-2(4)
C9	1377(3)	7909(4)	6418(3)	46(2)	49(4)	18(2)	26(5)	-14(3)	-8(5)
C10	2027(2)	4378(4)	5956(3)	18(2)	42(4)	28(3)	-7(4)	-9(3)	3(5)
O5	5000*	560(8)	2500*	106(6)	210(12)	89(5)	0	-81(9)	0

* Coordinate determined by space group symmetry

Table 19

FINAL POSITIONAL AND THERMAL PARAMETERS (x 10^3) FOR THE HYDROGEN ATOMS OF $Cu(H_2O)(ASCACHOPY)Cl \cdot \frac{1}{2}H_2O$

ATOM	BONDED TO	DISTANCE, Å	X	Y	Z	B (Å^2)
H1	O2	0.80	28	496	382	5.0
H2	O2	1.17	44	351	418	5.0
H3	C3	1.11	104	821	248	3.3
H4	C4	1.08	73	1037	288	3.7
H5	C9	0.90	124	870	641	3.8
H6	C9	1.01	107	731	678	3.8
H7	C9	1.02	187	773	682	3.8
H8	C7	0.96	139	1155	576	4.0
H9	C7	1.02	71	1255	559	4.0
H10	C7	1.05	53	1108	590	4.0
H11	N4	0.61	220	382	703	3.6
H12	N4	0.74	231	302	665	3.6
H13	N3	0.95	173	594	669	3.3

Table 20
INTRAMOLECULAR BOND DISTANCES AND ANGLES AND SHORT INTERMOLECULAR CONTACTS FOR $\mathrm{Cu(H_2O)(ASCACHOPY)Cl\cdot\frac{1}{2}H_2O}$ WITH THEIR ESTIMATED STANDARD DEVIATIONS IN PARENTHESES

(a) Bond Distances (Å)

Cu-Cℓ	2.253(1)	C1-C2	1.439(6)
Cu-O1	1.956(3)	C1-C8	1.473(6)
Cu-O2	2.374(3)	C2-C3	1.403(6)
Cu-O3	1.887(3)	C3-C4	1.366(7)
Cu-N1	1.966(3)	C4-C5	1.398(6)
O1-C10	1.251(6)	C5-C6	1.484(6)
O3-C2	1.308(6)	C6-C7	1.490(7)
N1-C8	1.288(6)	C6-O4	1.222(6)
N1-N3	1.392(5)	C8-C9	1.501(6)
N2-C1	1.340(6)	N3-C10	1.371(6)
N2-C5	1.325(6)	C10-N4	1.309(6)

(b) Bond Angles (°)

Cℓ-Cu-O1	91.6(1)	O3-C2-C1	125.5(4)
Cℓ-Cu-O2	96.0(1)	O3-C2-C3	118.2(4)
Cℓ-Cu-O3	92.9(1)	C1-C2-C3	116.2(4)
Cℓ-Cu-N1	166.1(1)	C2-C3-C4	121.1(4)
O1-Cu-O2	92.7(1)	C3-C4-C5	118.8(4)
O1-Cu-O3	172.2(1)	N2-C5-C4	121.7(4)
O1-Cu-N1	82.3(1)	N2-C5-C6	117.1(4)
O2-Cu-O3	93.2(1)	C4-C5-C6	121.2(4)
O2-Cu-N1	96.7(1)	C5-C6-C7	118.5(4)
O3-Cu-N1	91.9(1)	C5-C6-O4	119.7(4)
Cu-O1-C10	113.0(3)	C7-C6-O4	121.8(4)
Cu-O3-C2	127.6(3)	N1-C8-C1	119.0(4)
Cu-N1-C8	131.6(3)	N1-C8-C9	122.2(4)
Cu-N1-N3	109.8(2)	C1-C8-C9	118.9(4)
C1-N2-C5	120.8(4)	N1-N3-C10	114.6(3)
N2-C1-C2	121.2(4)	O1-C10-N3	119.9(4)
N2-C1-C8	114.7(4)	O1-C10-N4	123.0(4)
C2-C1-C8	124.1(4)	N3-C10-N4	117.2(4)

Table 20 - continued

(c) Short Intermolecular Contacts (Å)

ATOM A	EQUIV. POS.	ATOM B	EQUIV. POS.	DIST
N3	X,Y,Z	Cℓ	X,-Y,½+Z	3.346(4)
O4	X,Y,Z	O2	X,1+Y,Z	2.802(5)

Table 21

LEAST-SQUARES PLANES AND DEVIATIONS FOR $Cu(H_2O)(ASCACHOPY)Cl \cdot \frac{1}{2}H_2O$

The title of the planes are followed by the deviations (x 10^3 Å) of the atoms listed on the left. Asterisks denote deviations of atoms defining the plane. The equation of the plane is of the form ax+by+cz=d, where d is the distance (Å) from the origin. The dihedral angles are given in degrees and decimal fractions.

Plane 1. Plane Through the Base of the Square Pyramid

Plane 2. Plane Through Cu,O1,C10,N3,N1

Plane 3. Plane Through Cu,O3,C2,C1,C8,N1

Plane 4. Plane Through the Pyridine Ring

	Plane 1	Plane 2	Plane 3	Plane 4
Cu	-166	-28*	-15*	-5
Cℓ	58*	390	460	532
O1	-63*	24*	126	90
O2	-2542	-2395	-2376	-2359
O3	-63*	105	26*	75
N1	73*	37*	7*	-42
N2				-2*
N3		-31*		
C1			6*	-8*
C2			-23*	12*
C3				-7*
C4				-3*
C5				7*
C8			-2*	
C10		-2*		
a	0.9417	0.9549	0.9694	0.9583
b	0.3323	0.2957	0.2448	0.2440
c	0.0529	-0.0275	-0.0180	-0.0540
d	5.0796	4.2404	4.0328	3.7810

Dihedral Angles Between Planes

Plane A	Plane B	Angle
1	2	5.12
1	3	6.65
1	4	8.10

Table 21 - continued

Plane A	Plane B	Angle
2	3	3.08
2	4	3.41
3	4	2.06

Table 22

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $Cu(H_2O)(ASCACHOPY)Cl \cdot \frac{1}{2}H_2O$

The structure factors for the reflection (HKL) are listed to the right of the appropriate L value under the corresponding H and K value. FO and FC refer to F_{obs} and F_{calc} respectively.

```
    L    FO     FC

H=    0,  K=    0

    2  1280   1572
    4   747   -751
    6   122   -173
    8   913   -945
   10   314   -285
   12   304    309
   14   -27     49
   16   353    366

H=    2,  K=    0

    0  1108  -1275
    2  1072   1122
    4   560    564
    6   318   -271
    8   264    292
   10   602   -616
   12   342   -236
   14    54     28
  -14    82     50
  -12    45     31
  -10   627    629
   -8   685    676
   -6   864   -795
   -4    52   -119
   -2  1183  -1153

H=    4,  K=    0

    0  1135  -1191
    2   655   -645
    4   259    217
    6   294   -277
    8    31     -1
   10   947    945
   12   667    646
   14   -27     14
  -14   486   -513
  -12   214   -199
  -10   244   -241
   -8   188   -184
   -6   445    445
   -4    31     25
   -2  1323  -1261

H=    6,  K=    0

    0   536    529
    2   685    694
    4    46    -20
    6   469   -482
    8   321   -322
   10   796   -819
   12   299   -289
   14    63     69
  -14   597    611
  -12   102    112
  -10   240    227
   -8   162    167
   -6   991   -985
   -4   432   -394
   -2   349    332

H=    8,  K=    0

    0   591   -591
    2   434   -428
    4   932    886
    6   548    550
    8   251    244
   10   -28     33
   12   412   -391
   14    38    -22
  -14   307   -304
  -12   200    214
  -10    66     40
   -8   686    665
```

```
    L    FO     FC

   -6   999    964
   -4   403   -401
   -2   733   -719

H=   10,  K=    0

    0   197    162
    2   234   -231
    4   324   -323
    6   139    141
    8   -27     39
   10   440    441
   12   762    774
  -12   356   -354
  -10   165   -124
   -8   241   -237
   -6   308    302
   -4   833    822
   -2   100     99

H=   12,  K=    0

    0   -26     49
    2   304    306
    4   334    340
    6   178   -191
    8   221   -213
   10   566   -568
  -10   153   -148
   -8   327   -322
   -6   654   -677
   -4   399   -381
   -2   142    149

H=   14,  K=    0

    0   104   -110
    2   161   -159
    4    68    -68
    6   336    334
    8   113     99
   -8   215    214
   -6   401    399
   -4   117    115
   -2   350   -350

H=   16,  K=    0

    0   132   -134
    2   181   -173
    4   239   -249
    6   320   -333
   -6   -26      8
   -4   236    253
   -2   362    376

H=    1,  K=    1

    0   377   -349
    1   327   -333
    2   299   -336
    3   356   -322
    4    92     76
    5   274    236
    6   218    197
    7    36    -12
    8   448    466
    9    84     81
   10   823    862
   11   358    368
   12   338    339
   13   -27      1
   14   162    160
   15    87    -85
  -15   172   -185
  -14   383   -398
  -13    64    -53
  -12   472   -476
  -11   363    373
  -10   695   -687
```

```
    L    FO     FC

   -9   143   -145
   -8   -21      9
   -7   267   -249
   -6   919    937
   -5   335    338
   -4   279    305
   -3   158    105
   -2   263    237
   -1   442   -435

H=    3,  K=    1

    0  1294   1460
    1   473   -435
    2   990   1000
    3   175    131
    4   818   -766
    5   573   -504
    6    82     31
    7   255   -254
    8   502   -511
    9    73     92
   10   441   -446
   11   166   -173
   12   188    187
   13   -27    -40
   14   -27     45
   15   134   -146
  -15   175    177
  -14   235    236
  -13    87     81
  -12   -27     -4
  -11   145   -149
  -10   188    181
   -9   103     91
   -8   736   -717
   -7   617   -565
   -6   730   -736
   -5   711   -697
   -4    62    -70
   -3   940    948
   -2   233    226
   -1    50    -60

H=    5,  K=    1

    0  2298  -2652
    1  1318   1279
    2   490   -458
    3   160   -141
    4   447    457
    5    75    -73
    6    68     89
    7   144   -126
    8   523    506
    9   105    -98
   10   183   -148
   11   268   -264
   12   794   -760
   13   182   -176
   14    48    -29
   15   165    170
  -15   183   -179
  -14    58    -68
  -13   -29    -13
  -12   142    135
  -11   -28     17
  -10   201    212
   -9   279   -238
   -8   674    665
   -7   264    235
   -6   108    102
   -5   206   -173
   -4   302   -285
   -3   399   -400
   -2   806   -812
   -1  1566   1554

H=    7,  K=    1
```

```
    L    FO     FC

    0   228    228
    1   239    215
    2   832   -819
    3    64    -58
    4   694   -688
    5   137   -140
    6    56     55
    7   -23     -2
    8   -25     37
    9    81     77
   10   859    867
   11   282    283
   12   618    604
   13   101    104
   14   194   -195
  -14   194   -186
  -13   110   -105
  -12   309   -318
  -11   -27     38
  -10   268   -267
   -9   341    332
   -8   157   -154
   -7   232    249
   -6   863    850
   -5   260    243
   -4   744    722
   -3    56    -52
   -2   507    488
   -1   238   -214

H=    9,  K=    1

    0   640    616
    1   385   -374
    2   514    524
    3   176    163
    4   -23     11
    5   122    126
    6   322   -314
    7   122   -136
    8   248   -237
    9   213    204
   10   330   -327
   11   303    307
   12    83    -89
   13   205    200
  -13   -27     20
  -12   176    163
  -11   -28      0
  -10   119   -116
   -9   105   -102
   -8   210   -191
   -7   145   -135
   -6   778   -754
   -5   223   -217
   -4   192   -188
   -3   304   -270
   -2   920    892
   -1   625   -620

H=   11,  K=    1

    0    44    -50
    1   189    183
    2   133   -129
    3   -25     26
    4   221    213
    5    89    102
    6   508    493
    7    68     72
    8    43    -47
    9   269   -266
   10   -28      9
   11   190   -194
   12    40    -15
  -12   144    144
  -11   112    105
  -10   144    140
   -9    90     89
   -8   -27      7
   L    FO     FC       L    FO     FC       L    FC     FC       L    FO     FC

  -7    44    -64      15   259   -376       8   314   -323      -1   977   -948
  -6   437    440                              9   373    365
  -5    71    -57    H=   2, K=      2      10   291   -292    H=  12, K=      2
  -4   173   -168                             11   -28     49
  -3   126   -106       0   625   -659      12   -28     47       0   330    322
  -2   525   -520       1    83    105      13    77     61       1    89    -95
  -1   -24    -24       2   306    288      14    78     83       2   328    341
                        3   753    771     -14   294    297       3   130   -126
H=  13, K=      1       4   793    821     -13    41    -12       4   190    181
                        5   559   -550     -12   112     98       5   -27     -9
   0   -26    -14       6   938    949     -11   398   -403       6   189   -187
   1   151   -153       7   475   -440     -10   191    186       7   169   -171
   2    57     61       8   453    438      -9   -24     11       8   223   -213
   3   -27     29       9    61    -69      -8   306   -304       9   -28     37
   4   551   -551      10   811   -827      -7    86     94      10   225   -232
   5   157   -156      11   606   -613      -6   947   -942      11   155    150
   6   455   -455      12   610   -617      -5   372   -360     -11   -26    -28
   7    88    -87      13    86    -93      -4    44    -55     -10   -27    -19
   8    49     53      14    63    -60      -3   286    290      -9   271   -286
   9   -28     43      15   388    401      -2   277    289      -8    86    -77
  10    75     59     -15   205   -212      -1   147    152      -7   -28    -12
 -10   148   -152     -14    89     85                           -6   282   -280
  -9   -27     21     -13   110    108    H=   8, K=      2      -5    56     29
  -8   169   -152     -12   453    457                           -4   475  --480
  -7   229    234     -11   239   -246       0   751   -744      -3   109   -110
  -6   205   -189     -10   567    561       1   705    685      -2    46    -55
  -5    80     80      -9   321   -302       2   413   -409      -1   163    149
  -4   377    383      -8   263    284       3   156   -133
  -3   125    140      -7   293   -298       4   857    833    H=  14, K=      2
  -2   295    287      -6   556   -532       5   600    560
  -1   -27    -19      -5   848   -817       6   594    550       0   540   -541
                       -4   424   -419       7   315    313       1   236    246
H=  15, K=      1      -3   142   -141       8   153    151       2   119   -115
                       -2   918  -1004       9   261   -260       3   168    167
   0   227    216      -1   269    264      10    59     38       4   243    255
   1   108    122                             11   258    254       5   -27     33
   2   218    221    H=   4, K=      2      12   245   -243       6   366    372
   3   -28     14                             13   -26     38       7    45     34
   4   309    323       0   555    555     -14   142   -143       8   151    146
   5   177    176       1    89     76     -13   117   -120       9   176   -187
   6   -27    -20       2   428   -476     -12   222    229      -9   150    164
   7   -26    -12       3   232   -230     -11   243    239      -8   191    201
   8   234   -240       4   423   -430     -10   282    284      -7    43    -42
  -8   114   -122       5    74     85      -9    84    -61      -6   224    232
  -7   -27    -29       6   244   -246      -8   478    481      -5    61    -35
  -6   244   -262       7    46     72      -7    45    -13      -4   -27    -11
  -5   104    113       8   226    233      -6   212    202      -3   -28    252
  -4   399   -415       9   209   -215      -5   116    127      -2   617   -653
  -3   -28    -26      10   450    428      -4   370   -355      -1   256    275
  -2   -28     12      11    80     70      -3   621   -639
  -1   107    121      12   103     94      -2   426   -432    H=  16, K=      2
                       13   315   -301      -1   409    416
H=  17, K=      1      14    43    -49                            0    91   -106
                       15   230   -237    H=  10, K=      2       1   132   -146
   0   193   -192     -15   111   -105                            2   127   -145
   1    48    -35     -14   362   -367       0   556    523       3    41    -45
   2   -26    -30     -13   -29    -32       1   733   -709       4   170   -169
   3    87     92     -12   486   -453       2    69    -69       5    63     52
  -4   112    113     -11   426    417       3    88    -60      -6   -26     26
  -3    64     75     -10   504   -493       4   693   -672      -5   144    153
  -2   159   -174      -9   282    264       5   512   -477      -4   257    281
  -1    51    -53      -8    58    -36       6   265   -258      -3   -27     -1
                       -7   269    254       7   125    119      -2   244    256
H=   0, K=      2      -6   605    591       8   155    155      -1   -28     16
                       -5   779    762       9   232    222
   0  1078   1158      -4   283    276      10   189    184    H=   1, K=      3
   1   128    105      -3   129   -140      11   124   -115
   2   404    473      -2    83     94      12   298    299       0   823   -858
   3   299   -321      -1    90     94     -13   118    119       1   390    417
   4   121     67                            -12   271   -261       2   747   -827
   5    70     47    H=   6, K=      2     -11    97    -74       3   523   -541
   6   606   -612                            -10   210   -209       4   596   -604
   7   520    490       0   436    427      -9   279    275       5   578    596
   8   780   -808       1   440   -438      -8    43    -24       6   188   -182
   9   262   -249       2   570    581      -7    93     89       7   192    200
  10    93     67       3   387    366      -6   285    287       8   245    272
  11   263    279       4   112   -104      -5   111    112       9    48    -49
  12   500    521       5   118   -122      -4   437    435      10   359    358
  13   249    236       6   518   -510      -3   198    187      11   112    114
  14   279    301       7    57    -63      -2   376    361      12   138    143
```

```
   L    FO    FC

  13   215  -222
  14    40    33
  15    56   -56
 -15   258  -272
 -14    46   -46
 -13   243  -235
 -12   141  -117
 -11   364   330
 -10   380  -394
  -9    66   -80
  -8   233   227
  -7   224   234
  -6  1179  1214
  -5   528   518
  -4   712   737
  -3   512  -558
  -2    98   -54
  -1    45    14

H=    3,  K=    3

   0   326   342
   1   260  -293
   2   524   573
   3   198  -177
   4   184  -187
   5  1036 -1059
   6   491  -478
   7   394  -395
   8   217  -226
   9    99   103
  10 . 136  -134
  11    81   -76
  12   157  -150
  13   247   249
  14   242   248
  15   141  -144
 -15   361   366
 -14   149   156
 -13    91  -104
 -12   362   354
 -11   785  -808
 -10   165   149
  -9   103  -104
  -8   601  -617
  -7   137  -118
  -6   560  -559
  -5   153  -144
  -4    29     4
  -3   871   901
  -2   172   219
  -1   341  -308

H=    5,  K=    3

   0   219  -219
   1   293   316
   2   304  -300
   3   330   327
   4   751   749
   5   773   732
   6  1184  1172
   7   483  -476
   8   217   201
   9   187  -176
  10   242  -222
  11    88    78
  12   344  -325
  13    91   -75
  14   357  -369
 -14   214  -231
 -13   206   194
 -12   112  -116
 -11   351   330
 -10   269   248
  -9   394  -359
  -8   306   301
  -7    38   -31
  -6    45    -7
  -5   320  -314
```

```
   L    FO    FC

  -4   300  -296
  -3   354  -343
  -2   125  -146
  -1   635   601

H=    7,  K=    3

   0    78   -68
   1    77   -52
   2   345  -352
   3   114  -114
   4   851  -852
   5   264   258
   6   525  -519
   7   592   563
   8   162   156
   9    43     2
  10   387   378
  11    87   -96
  12   222   219
  13    42   -11
  14    55   -13
 -14    46   -52
 -13   132   128
 -12   525  -529
 -11   278   279
 -10   455  -448
  -9   411   397
  -8   111  -108
  -7    61   -50
  -6   240   236
  -5   331   326
  -4   809   822
  -3   356   351
  -2   655   654
  -1   475  -484

H=    9,  K=    3

   0   515   515
   1    63    28
   2   331   334
   3   141  -128
   4   191  -191
   5   218  -213
   6   419  -407
   7   200  -200
   8   292  -287
   9   263   258
  10    85   -80
  11   -28    47
  12   -27    44
  13    99    85
 -13    46   -19
 -12   407   408
 -11   267  -273
 -10   -28     7
  -9   430  -437
  -8   328  -322
  -7   -26   -32
  -6   383  -376
  -5   273  -268
  -4   230  -226
  -3    40   -19
  -2   348   334
  -1   391   392

H=   11,  K=    3

   0   219  -220
   1   475   483
   2    62 .  -62
   3    58   -46
   4   323   306
   5   -26   -29
   6   356   359
   7   -27    22
   8   154   154
   9   294  -291
  10   -27    33
```

```
   L    FO    FC

  11   -27   -36
 -12    59    56
 -11   209   219
 -10   264   261
  -9   250   237
  -8   349   349
  -7   233  -240
  -6    85    73
  -5   139  -132
  -4   316  -309
  -3   180  -168
  -2   256  -250
  -1   -25    20

H=   13,  K=    3

   0   188   199
   1   575  -587
   2    68   -61
   3   -28    47
   4   302  -302
   5    82   -49
   6   171  -160
   7    99   -96
   8   -27    33
   9   198   198
 -10   215  -221
  -9    92    76
  -8   141  -146
  -7   236   242
  -6   109   107
  -5   -28   -30
  -4    86    71
  -3   -27    37
  -2    74    67
  -1   387  -393

H=   15,  K=    3

   0   -28    -7
   1   358   371
   2   233   238
   3   -27    -6
   4   153   150
   5    71    83
   6    54   -46
   7    47   -53
  -7    81   -90
  -6   202  -209
  -5   104   102
  -4   150  -159
  -3   -28   -27
  -2   218  -224
  -1   266   289

H=   17,  K=    3

   0   238  -271
  -1   -26 .   56

H=    0,  K=    4

   0   162   206
   1   437   406
   2   419   418
   3   228  -242
   4   504  -492
   5  1110 -1141
   6  1081 -1115
   7   -22     2
   8   221  -239
   9    51    51
  10    93   -96
  11   183   188
  12   113   118
  13   197   189
  14   401   426
  15   122  -122

H=    2,  K=    4
```

```
   L    FO    FC

   0   364   336
   1   274  -257
   2   172   160
   3   688   735
   4   715   742
   5   248   243
   6   678   710
   7   519  -526
   8    82   -63
   9   192  -209
  10   109  -102
  11   241  -247
  12   115  -115
  13    48   -48
  14   172  -162
 -15   113  -108
 -14   267  -265
 -13   145   137
 -12   308   289
 -11   -27    -3
 -10   354   364
  -9   -24   -23
  -8   317   313
  -7    42   -40
  -6   335   333
  -5   857  -889
  -4   772  -812
  -3   721  -705
  -2   699  -745
  -1   176   161

H=    4,  K=    4

   0   470  -473
   1   410  -406
   2   149  -156
   3    70   -78
   4   364  -389
   5   803   807
   6   407  -404
   7   680   680
   8    83    78
   9   225  -235
  10   124   129
  11    82    78
  12   120    91
  13   137  -124
  14    42   -30
 -14    54   -54
 -13   255  -252
 -12   352  -331
 -11   186   179
 -10    90   -76
  -9   489   484
  -8   287   261
  -7    79    87
  -6   452   446
  -5   352   364
  -4   768   794
  -3   394  -397
  -2    93   108
  -1   784  -824

H=    6,  K=    4

   0   501   526
   1   556  -550
   2   517   498
   3    35    45
   4   232   240
   5   441  -422
   6   190  -195
   7   111  -107
   8   305  -308
   9   262   265
  10   121  -127
  11   -27    13
  12    49   -65
  13   138   135
```

```
   L    FO     FC

 -14    49     46
 -13   234    245
 -12   222    217
 -11   452   -457
 -10    65    -73
  -9   351   -338
  -8   497   -497
  -7   233    222
  -6   419   -411
  -5   264    265
  -4   236   -245
  -3   493    475
  -2    60     34
  -1   131    -86

H=    8,  K=    4

   0   215   -228
   1   419    438
   2    56     51
   3   149    135
   4   318    316
   5   370    372
   6   513    506
   7    94    106
   8   128    115
   9   238   -234
  10   207   -203
  11    63    -61
  12   114   -120
  13   176   -179
 -13    52     44
 -12   243   -242
 -11   460    461
 -10   188    189
  -9   -27     12
  -8   396    396
  -7   211   -204
  -6   -25     16
  -5   -24     38
  -4    75    -64
  -3   146   -138
  -2   182   -193
  -1   438    423

H=   10,  K=    4

   0   193   -181
   1   516   -498
   2   363   -360
   3   202   -202
   4   311   -303
   5    60    -43
   6   357   -362
   7   434    425
   8    82     71
   9   161    157
  10   232    230
  11   188   -195
 -12   136   -131
 -11   254   -258
 -10   428   -424
  -9   141    132
  -8   -28      5
  -7   165    161
  -6   239    238
  -5    81     83
  -4   182    180
  -3   250    249
  -2   282    263
  -1   213   -202

H=   12,  K=    4

   0   257    267
   1    77     64
   2   213    199
   3   280   -271
   4   195    190
   5   237   -250
```

```
   L    FO     FC

   6   179    172
   7   298   -303
   8   175   -175
   9    39     42
  10   114   -108
 -10   214    219
  -9   391   -393
  -8   261   -268
  -7   126   -131
  -6   169   -170
  -5    85     86
  -4   237   -242
  -3    58    -56
  -2   222   -213
  -1   285    285

H=   14,  K=    4

   0   340   -354
   1   118    123
   2    56    -48
   3   125    120
   4   113    125
   5   169   -165
   6   190    196
   7   -27     47
  -8   194    207
  -7   189   -194
  -6   -27     -7
  -5   148   -147
  -4    42    -25
  -3    92     88
  -2   189   -194
  -1   131   -136

H=   16,  K=    4

   0   142    151
   1   228   -242
   2   157   -167
   3    61    -46
  -4   213    231
  -3   -26      1
  -2   179    182
  -1   -27     36

H=    1,  K=    5

   0   341    304
   1   586   -602
   2   269   -265
   3   279   -275
   4   741   -807
   5   538    574
   6   -22     10
   7   231    249
   8    55     67
   9   202    200
  10   -26      9
  11    51     69
  12   290    294
  13   235   -236
  14   212   -221
 -14   103   -113
 -13   189   -201
 -12   388   -394
 -11   193    200
 -10   129    135
  -9   166    167
  -8   214    212
  -7   279    287
  -6   252    244
  -5   136    132
  -4   473    523
  -3   260   -259
  -2    95    112
  -1   330   -368

H=    3,  K=    5
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```
   L    FC     FC

   0   133    -91
   1   -19    -22
   2   335    329
   3   698   -714
   4   284    302
   5   817   -848
   6   659   -674
   7    74    -53
   8   330   -324
   9   312    317
  10    33    -13
  11   220    232
  12   -27     38
  13   238    242
  14   426    437
 -14   174    174
 -13   -27     14
 -12   157    167
 -11   274   -268
 -10   245   -239
  -9   348   -349
  -8    80    -89
  -7   177   -168
  -6   421   -420
  -5   442    449
  -4   517   -510
  -3   456    477
  -2    50     27
  -1   258   -233

H=    5,  K=    5

   0    92     -2
   1   453    449
   2   273    277
   3   357    359
   4   320    324
   5   239    222
   6   636    584
   7   492   -462
   8    61     47
   9   227   -223
  10   -28    -17
  11   -29    -30
  12    69    -67
  13    73    -76
 -13   231    234
 -12   122    110
 -11   398    381
 -10   536    505
  -9   128    120
  -8   169    173
  -7   431   -407
  -6   567    526
  -5   842   -835
  -4   211    187
  -3   235   -238
  -2   692   -689
  -1   412    416

H=    7,  K=    5

   0   526   -518
   1    43    -18
   2   379   -366
   3    36    -19
   4   303   -303
   5   143    135
   6   392   -380
   7   409    392
   8   246    243
   9    43     43
  10   103     88
  11    85   -100
  12   -26    -33
 -13   105   -108
 -12   377   -370
 -11    67    -77
 -10   380   -382
  -9   358    345
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   L    FO     FC

  -8   236    236
  -7   319    316
  -6   107     91
  -5   166    164
  -4   428    422
  -3   188    170
  -2   503    479
  -1   236   -240

H=    9,  K=    5

   0   576    576
   1   126    126
   2    95     91
   3   103    -99
   4   232    233
   5   212   -212
   6   163    168
   7   469   -466
   8   373   -369
   9   -27     12
  10    48    -17
  11   177    180
 -12   132    130
 -11   268   -262
 -10   131   -143
  -9   454   -458
  -8   414   -415
  -7   235    222
  -6   190   -184
  -5   206    196
  -4   385   -372
  -3   128    123
  -2   -25    -26
  -1   471    475

H=   11,  K=    5

   0   424   -425
   1   426    409
   2    78     85
   3   298    299
   4   108     99
   5   110    104
   6   115    108
   7   -27     -2
   8   195    194
   9   258   -254
  10   162   -162
 -10   104    110
  -9    69     58
  -8   115    110
  -7   522   -529
  -6   152   -137
  -5   322   -324
  -4    59     39
  -3   257   -254
  -2   226   -211
  -1   149   -155

H=   13,  K=    5

   0   138    124
   1   341   -343
   2   266   -263
   3    84    -82
   4   138   -147
   5   170    160
   6    88    -92
   7   149    148
   8    57    -58
  -8   132   -116
  -7   215    204
  -6   239    239
  -5    69     62
  -4   172    164
  -3   -28      7
  -2   200    211
  -1   189   -191
```

```
   L    FC     FC

H=  15,  K=    5

   0   158    158
   1   142    146
   2   227    232
   3    61    -57
   4   -26    -43
  -5    81     64
  -4   -26      6
  -3    50     50
  -2   -27      5
  -1    54     57

H=    0,  K=    6

   0   -20     31
   1   148   -144
   2   200    212
   3   336   -367
   4   210   -218
   5   385   -398
   6   419   -425
   7    86     88
   8   175   -192
   9   352    357
  10   428   -428
  11   312    315
  12   -27    -22
  13   186    197

H=    2,  K=    6

   0   368    350
   1   150    170
   2   337    320
   3   310    334
   4   399    412
   5   144    144
   6   398    411
   7   311   -315
   8    84    -80
   9   325   -342
  10   100    112
  11   117   -100
  12   195   -201
  13    47    -36
 -13   275    292
 -12   247    239
 -11   404    414
 -10   293    297
  -9    52     43
  -8   136   -140
  -7   539   -549
  -6   205    215
  -5   621   -644
  -4   322   -329
  -3   428   -428
  -2   544   -534
  -1   123    138

H=    4,  K=    6

   0   531   -538
   1   451   -462
   2    73    -68
   3    37    -13
   4   519   -524
   5   178    165
   6   162   -156
   7   482    480
   8   340    338
   9   220    217
  10    52    -73
  11   189   -198
  12   123    105
  13   291   -302
 -13   169   -172
 -12   294   -310
 -11   161    156
```

```
   L    FO     FC

 -10   135    127
  -9   514    491
  -8   285    280
  -7   230    223
  -6    81    -70
  -5    73     78
  -4   628    647
  -3   212   -228
  -2   248    278
  -1   615   -639

H=    6,  K=    6

   0   182    202
   1   124    119
   2   131   -136
   3   395   -396
   4   335    333
   5   388   -379
   6   121   -111
   7   125   -119
   8   276   -273
   9    92    100
  10   240    248
  11   310    300
  12    55     68
 -12   172    173
 -11   373   -367
 -10   225   -221
  -9   104    -90
  -8    53     38
  -7   454    454
  -6   181    181
  -5   394    389
  -4   453   -461
  -3   300    301
  -2   174    166
  -1   -37    561

H=    8,  K=    6

   0   182   -186
   1   239    236
   2   164    168
   3   468    462
   4    98    -96
   5   106     98
   6   301    285
   7   164   -160
   8   256    250
   9   209   -205
  10    90    -74
  11   110   -103
 -11   156    151
 -10   271    264
  -9   140    128
  -8    53     22
  -7   199   -203
  -6    53    -23
  -5   457   -442
  -4   103     95
  -3   323   -314
  -2   445   -437
  -1    72    -81

H=  10,  K=    6

   0    89    -85
   1   386   -385
   2   329   -325
   3    65    -68
   4   -27      6
   5   260    257
   6   189   -189
   7   272    263
   8    96   -106
   9   126    124
  10   131    117
 -10   360   -360
  -9   150   -143
```

```
   L    FO     FC

  -8   198   -203
  -7   228    222
  -6    77    -84
  -5   407    393
  -4    63    -56
  -3   -28    -30
  -2   328    317
  -1   344   -334

H=  12,  K=    6

   0   429    438
   1   124    122
   2   360    352
   3   217   -218
   4   114   -117
   5   372   -366
   6    52     -3
   7   205   -208
   8   239   -244
  -8    61    -72
  -7    60    -72
  -6    83    -82
  -5   210    214
  -4    46     46
  -3   268    273
  -2   -28    -39
  -1   232    219

H=  14,  K=    6

   0   271   -274
   1    93     89
   2   -27     11
   3   209    214
   4   120    125
   5   131    131
  -5   321   -328
  -4    40    -33
  -3   150   -161
  -2    39    -33
  -1    43    -46

H=    1,  K=    7

   0    67    -60
   1   394   -418
   2   136   -133
   3   248    254
   4   443   -459
   5   184    186
   6   149    147
   7   402    412
   8   -27      6
   9   269    269
  10   232   -243
  11   297   -307
  12   115    118
 -12   114   -107
 -11    59     36
 -10   176    189
  -9   229    233
  -8   418   -427
  -7   129   -125
  -6   193   -199
  -5   222   -228
  -4   636    660
  -3    43    -42
  -2    84    -84
  -1   702   -739

H=    3,  K=    7

   0   167    172
   1    67    -57
   2    77     66
   3   576   -589
   4   262    264
   5   440   -452
   6    50    -43
```

```
   L    FO     FC

   7   415   -408
   8   -27    -31
   9   180    175
  10   200   -209
  11   445    450
  12   165   -174
 -12   153    143
 -11   286   -289
 -10   279   -277
  -9   345   -346
  -8    87     81
  -7   104     99
  -6    57    -53
  -5   443    431
  -4   224   -227
  -3   596    601
  -2   311    317
  -1   639    660

H=    5,  K=    7

   0    82     67
   1   465    487
   2   192    187
   3   235    232
   4   -26     18
   5   171   -170
   6   287    284
   7   239   -240
   8   304    307
   9   380   -361
  10   117    122
  11   251   -248
 -12    52     34
 -11   208    212
 -10   430    423
  -9   256    243
  -8   205    199
  -7   212   -202
  -6    51     57
  -5   472   -458
  -4   -25     13
  -3   146   -141
  -2   333   -343
  -1   173    180

H=    7,  K=    7

   0   466   -462
   1   327   -342
   2   438   -434
   3    90     67
   4   -27     15
   5   439    436
   6   124   -114
   7   290    282
   8   199    197
   9   275    278
  10   212    202
  11    60     40
 -11   -26     14
 -10   236   -226
  -9   -27    -16
  -8   -27      2
  -7   254    247
  -6   119   -124
  -5    53     43
  -4    55     48
  -3   219   -216
  -2   247    247
  -1   277   -267

H=    9,  K=    7

   0   378    371
   1   251    258
   2    41    -38
   3   301   -295
   4    73    -76
   5   382   -375
```

L	FO	FC
6	97	-98
7	224	-225
8	365	-373
9	100	-110
-10	60	50
-9	135	-142
-8	236	-239
-7	134	-128
-6	40	-7
-5	239	235
-4	127	-116
-3	320	310
-2	68	-48
-1	297	289

H= 11, K= 7

L	FO	FC
0	-28	24
1	154	147
2	161	159
3	274	265
4	241	-242
5	49	-33
6	54	-62
7	105	-104
-8	255	257
-7	85	-85
-6	52	-29
-5	446	-455
-4	49	-23
-3	349	-349
-2	85	-96
-1	122	-122

H= 13, K= 7

L	FO	FC
0	74	78
1	95	-92
2	-26	30
3	91	78
4	215	227
-5	260	271
-4	39	8
-3	52	-45
-2	64	65
-1	206	-199

H= 0, K= 8

L	FO	FC
0	78	-86
1	286	-298
2	89	89
3	271	-270
4	64	57
5	194	-195
6	83	-78
7	197	-194
8	236	-246
9	285	275
10	247	-266
11	319	320

H= 2, K= 8

L	FO	FC
0	-25	-3
1	888	934
2	-25	-4
3	363	375
4	-26	-39
5	94	-93
6	93	-94
7	-27	14
8	189	-187
9	457	-462
10	51	2
11	319	-329
-11	194	199
-10	212	213
-9	182	174
-8	162	165

L	FO	FC
-7	315	-303
-6	177	190
-5	202	-204
-4	126	-123
-3	222	-228
-2	188	-207
-1	149	126

H= 4, K= 8

L	FO	FC
0	180	-169
1	738	-715
2	-28	7
3	450	431
4	-28	-17
5	451	433
6	418	396
7	110	100
8	482	506
9	243	255
10	-26	-7
11	179	-187
-11	152	-159
-10	-26	21
-9	138	134
-8	-27	-5
-7	447	433
-6	80	-76
-5	97	-99
-4	214	202
-3	174	-154
-2	74	75
-1	565	-548

H= 6, K= 8

L	FO	FC
0	77	60
1	109	-97
2	-27	-20
3	423	-412
4	339	330
5	-27	5
6	72	69
7	175	-169
8	120	-122
9	77	-81
10	133	147
-10	149	-145
-9	323	-314
-8	125	-133
-7	113	-113
-6	-27	-14
-5	549	551
-4	63	-62
-3	422	419
-2	196	209
-1	321	317

H= 8, K= 8

L	FO	FC
0	88	-51
1	85	82
2	129	-132
3	-28	34
4	496	-490
5	88	-89
6	216	-211
7	123	120
8	71	53
9	178	-176
-9	123	128
-8	80	66
-7	120	-118
-6	45	-53
-5	429	-420
-4	42	39
-3	218	-208
-2	66	-66
-1	77	-77

L FO FC

H= 10, K= 8

L	FO	FC
0	40	-1
1	229	-232
2	260	-257
3	212	-211
4	131	-130
5	248	240
6	91	-91
7	379	371
-7	282	279
-6	177	173
-5	264	270
-4	47	-22
-3	210	-205
-2	78	84
-1	216	-215

H= 12, K= 8

L	FO	FC
0	194	200
1	105	121
2	380	383
3	-26	8
4	73	71
-4	74	86
-3	452	459
-2	-26	20
-1	134	134

H= 1, K= 9

L	FO	FC
0	122	134
1	282	-285
2	62	29
3	170	162
4	176	-180
5	97	-110
6	60	-46
7	308	314
8	178	182
9	116	128
10	57	42
-10	-25	8
-9	432	436
-8	57	-47
-7	390	386
-6	254	-259
-5	191	180
-4	359	-363
-3	-27	29
-2	130	-135
-1	641	-663

H= 3, K= 9

L	FO	FC
0	-28	27
1	95	-81
2	327	320
3	113	-102
4	521	491
5	91	100
6	-27	-1
7	197	-190
8	261	-273
9	255	247
-10	-24	40
-9	373	-373
-8	52	-50
-7	-27	-23
-6	81	76
-5	196	191
-4	91	98
-3	384	384
-2	61	-41
-1	539	553

H= 5, K= 9

L	FO	FC
0	-27	21

L	FC	FC
1	439	428
2	73	83
3	367	353
4	66	35
5	52	-36
6	-27	-36
7	97	-95
8	-26	-28
9	398	-393
-9	-26	-6
-8	98	100
-7	479	-469
-6	71	-78
-5	439	-432
-4	-27	-42
-3	-27	-27
-2	43	-40
-1	59	44

H= 7, K= 9

L	FO	FC
0	-27	9
1	531	-534
2	167	-163
3	202	-200
4	-27	-27
5	300	299
6	220	221
7	-26	46
8	187	185
-8	-25	25
-7	440	436
-6	105	104
-5	73	72
-4	71	-61
-3	385	-383
-2	-28	-53
-1	225	-234

H= 9, K= 9

L	FO	FC
0	103	-108
1	250	250
2	86	81
3	262	-262
4	42	-37
5	337	-331
6	172	-174
-6	-25	15
-5	290	293
-4	89	90
-3	312	311
-2	102	-103
-1	70	50

H= 11, K= 9

L	FO	FC
0	-26	-20
1	60	68
2	89	-84
-2	120	131
-1	159	152

H= 0, K= 10

L	FO	FC
0	76	-85
1	243	-240
2	55	-42
3	235	-239
4	94	109
5	232	-241
6	148	150
7	222	-225
8	43	36

H= 2, K= 10

L	FO	FC
0	-28	-40
1	579	588
2	51	44

```
   L    FO     FC       L    FO     FC       L    FO     FC       L    FO     FC

   3   367    367       7   224    223                           -2   301    315
   4    81    -81      -7   418    410   H=     8,  K=   10     -1   191   -176
   5    45    -45      -6   134    122
   6   141   -141      -5   182   -191      0   -26     34   H=     3,  K=   11
   7   166   -172      -4   112   -114      1   180    167
   8   -25     -1      -3   208   -201      2    56    -63      0    57    -61
  -8   144    150      -2   -26     18      3   364    364      1   -26     40
  -7   479   -479      -1   211   -197      4   -25     12      2    83    -86
  -6   174   -173                          -4    87    -88      3   240   -235
  -5   -27     12   H=     6,  K=   10     -3    94    -93      4   147   -143
  -4   229   -226                          -2   211    207     -5   229    221
  -3   265    275       0   134   -127     -1    39     -9     -4   119    112
  -2    50     -6       1   132    129                          -3   199    187
  -1   142    155       2   116    112   H=     1,  K=   11     -2   243   -242
                        3   338   -323                          -1   216    205
H=     4,  K=   10      4   134   -136      0    61     77
                        5   187   -176      1   235   -232   H=     5,  K=   11
   0   121    114       6   -25    -34      2    51    -48
   1   468   -471      -6   247    243      3   -26     -3      0   -25     23
   2    74    -78      -5    71     50      4   258    258      1   278    273
   3    55     51      -4   361    363      5   159    157      2   -25     19
   4   133    130      -3    69    -78     -5   -25     21      3   285    285
   5   315    305      -2   162   -175     -4   211   -206     -3    58    -65
   6    87     97      -1    79     82     -3   -26    -11     -2    49     36
```

FIGURE 8

Cu(H_2O)(ASCACHOPY)Cl Complex

The atomic numbering scheme and 50% probability thermal ellipsoids are shown. Hydrogen atoms are omitted for clarit

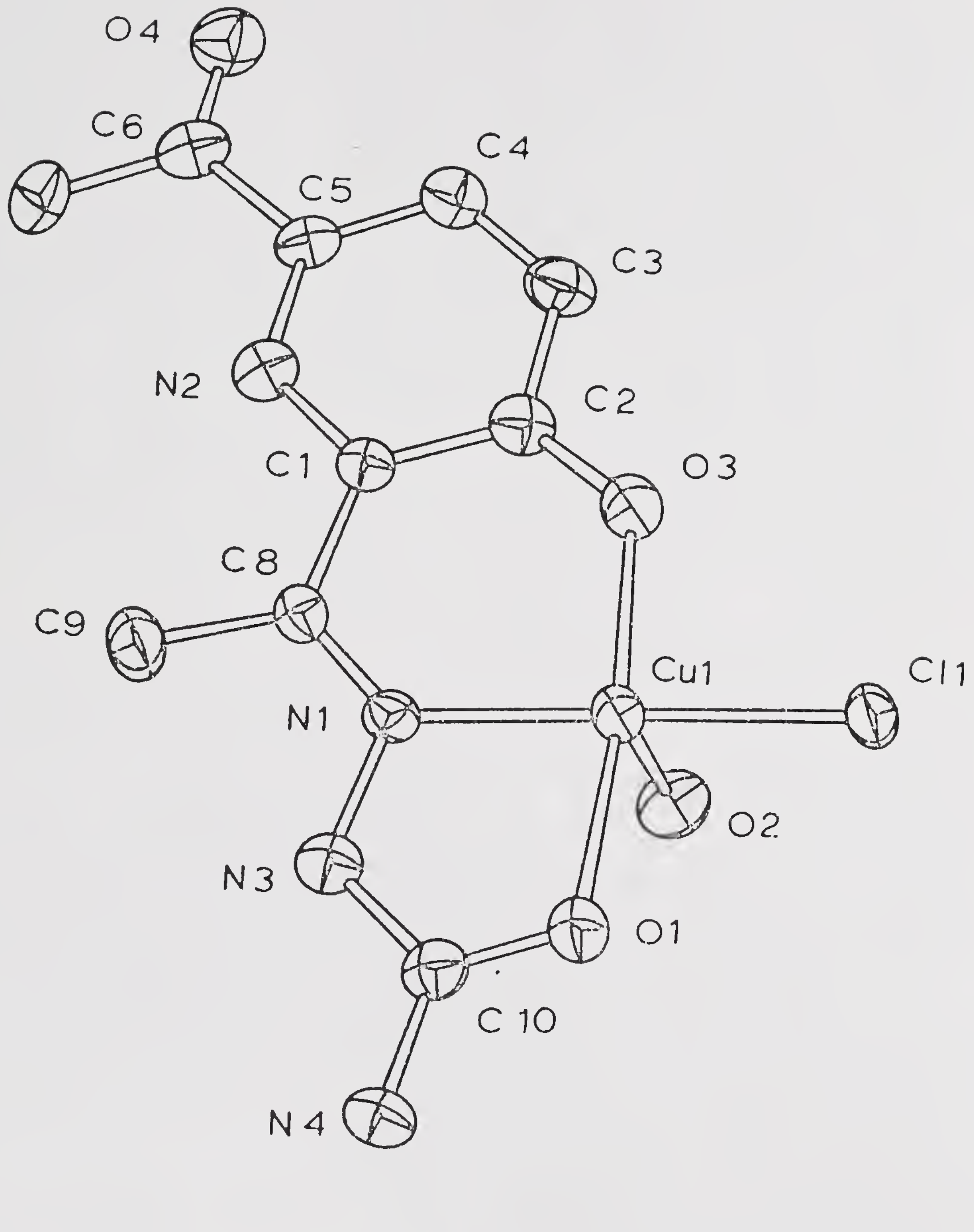
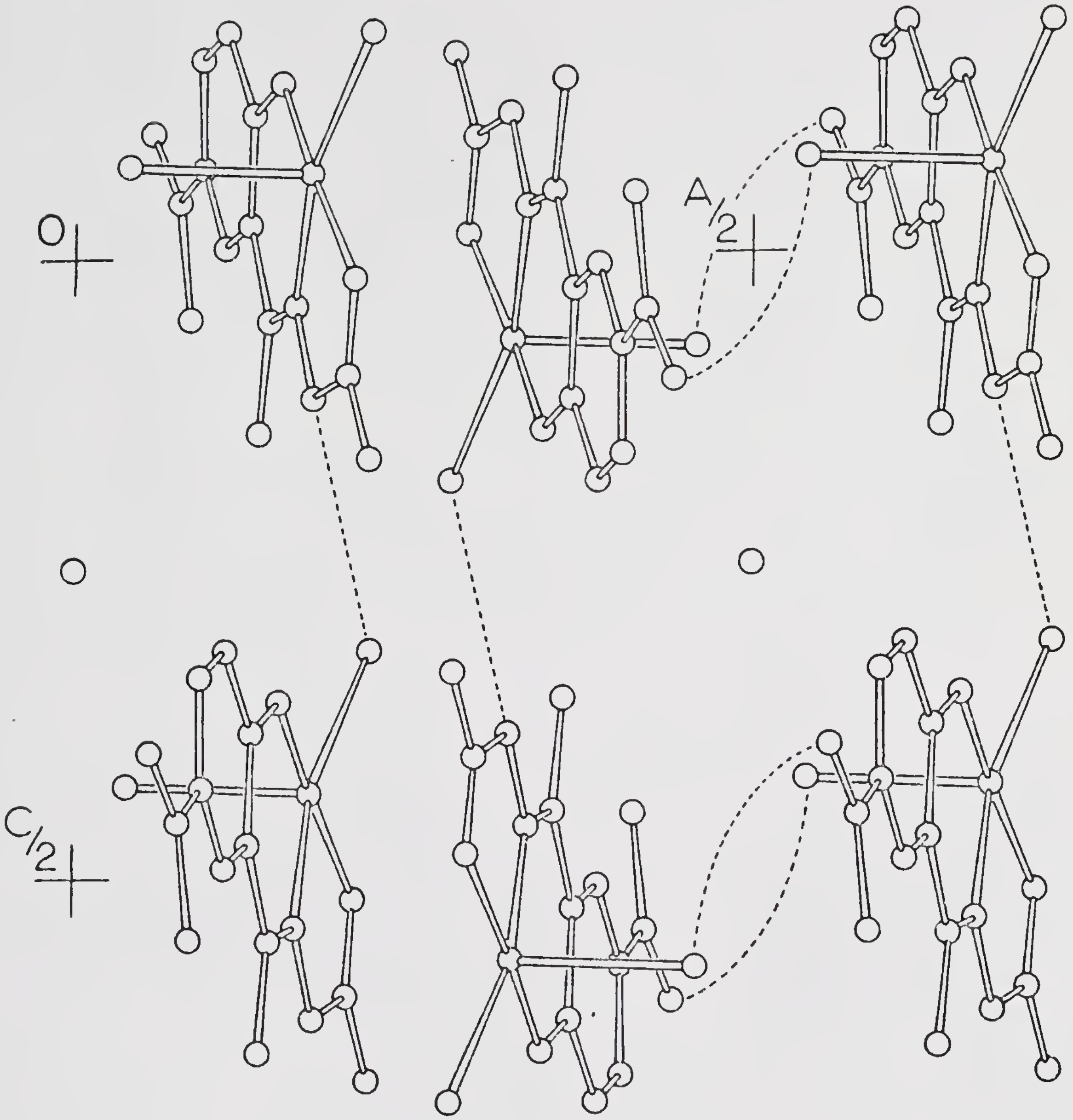

O4
C6
C7
C4
C5
C3
N2
C2
C1
O3
C8
C9
Cu1
Cl1
N1
O2
N3
O1
C 10
N 4

FIGURE 9

A PACKING DIAGRAM FOR $Cu(H_2O)(ASCACHOPY)Cl\cdot\frac{1}{2}H_2O$

The view is a projection along the b axis. The atomic numbering and hydrogen atoms are omitted for clarity. Isolated circles represent waters of hydration. Dotted lines represent hydrogen bonds listed in Table 20.


O
A/2
C/2

in Table 21. The observed and calculated structure factors are in Table 22. Figure 8 is an ORTEP[58] drawing of the molecular species showing the atomic numbering scheme. An ORTEP[58] packing diagram of the unit cell is illustrated in Figure 9.

Discussion

The square pyramidal coordination of the central copper atom is readily seen in Figure 8. Atoms Cℓ1, O1, O3, and N1 form the base and O2 occupies the apical position.

The most interesting feature of this complex is the oxidation which has occurred on the pyridine ring. The atom C2 is bonded to a phenolic oxygen atom, whereas in the starting DAP it is bonded to a hydrogen atom. Reactions in which oxygen plays a key role are well known,[84,85] and this oxidation does not occur when oxygen is excluded from the reaction mixture. The copper containing phenolase enzyme complex has been found to introduce hydroxyl into benzene rings using molecular oxygen.[86] Thus, it appears that this complex is an air oxidation product of the reaction.

A diversity of donor atoms surroundsthe copper ion. The apical water-copper bond distances of 2.374(3)Å is rather long,[87] but other square pyramidal complexes with comparable distances are known.[87,88] The copper-chlorine bond distance of 2.253(1)Å is identical within experimental error to previously reported values.[87] The bond distance of 1.887(3)Å for the hydroxo-copper bond is similar to the

Cu-O bond distance for many complexes with derivatives of salicylaldehyde.[65,87,89-91] Similarly, the Cu-N distance of 1.966(3)Å is within the range of values already found for Cu-imine nitrogen bonds.[65,87-91] Finally, the Cu-O (semicarbazide) distance of 1.956(3)Å is in agreement with earlier measurements.[73,87,90,91]

The angles about the coordination sphere are typical of square pyramidal copper(II) complexes.[87,88,90,91] The axial water-Cu-basal donor angles are all greater than 90°, indicating that the Cu atom lies above the plane of the square base. The deviation of the copper atom from the plane defined by the four basal atoms is 0.17Å. Such deviations are common among square pyramidal Cu(II) complexes.[90,92] The donor atoms defining the basal plane do not deviate greater than 0.07Å from this plane. Atoms Cℓ1 and N1 are above the plane by 0.06 and 0.07Å, while atoms O1 and O3 are below the plane by 0.07 and 0.06Å, respectively.

The bond lengths in the ligand are of the same magnitude as equivalent distances already determined.[65-67,73,89,90] The ligand functions as a tridentate chelating agent. Although the pyridine nitrogen and acetyl oxygan are available for coordination, the semicarbazone oxygen and amine nitrogen and the oxygen in the 3- position on the pyridine ring are the only coordinated atoms. A high degree of planarity is present in the ligand as evidenced by the small deviations from the least-squares planes of the chelate rings. The angles between these rings are also small. Thus the ligand differs greatly from DAPSC with respect to both composition and conformation but retains the planarity associated with DAPSC.

The packing diagram, Figure 9, shows the hydrogen bonding pattern of the molecules in the unit cell. The coordinated chloride hydrogen bonds to the NH and NH_2 groups of the semicarbazone residue. This interaction is not symmetrical however, the Cℓ-N distances being 3.16Å and 3.35Å for N3 and N4, respectively. Thus the major interaction occurs between Cℓ and N3, as shown. The other hydrogen bond present is situated near a center of symmetry. The apical water, O2, is hydrogen bonded to the acetyl portion of a neighboring molecule, and the apical water of the neighboring molecule is bonded to the acetyl group of the first molecule. These bonds are related by a center of symmetry at (½,½,0), as illustrated. There are no intermolecular contacts less than 3.5Å involving the Cu atom.

CHAPTER 5
COMPLEXES OF TRANSITION METAL NITRATES AND DAPSC

The remarkable results obtained from structural analysis of the complexes of DAPSC with transition metal chlorides encouraged extension of these studies to include complexes formed with transition metal nitrates. Water molecules occupy all apical positions in these complexes. Comparision of the chloride and nitrate complexes should allow determination of the effects of the axial chloride in the $[M(DAPSC)(H_2O)Cl]^+$ complexes. To avoid interference from the chloride ions present in SCA, a method of preparation involving preformed DAPSC was chosen. Thus an ethanolic slurry of the difficultly soluble DAPSC and a solution of the appropriate nitrate were mixed, heated, and stirred until complete dissolution of the DAPSC occurred. The structures of the products which crystallized from these mixtures are described in this chapter.

Structure Solution and Refinement for $[M(DAPSC)(H_2O)_2](NO_3)_2 \cdot H_2O$ (M=Ni,Mn)

The nickel position was calculated from a sharpened three-dimensional Patterson function. A Fourier synthesis phased on the nickel atom revealed the atoms in the coordination sphere. Subsequent Fourier syntheses yielded the positions of all other atoms. A difference Fourier synthesis at this point contained no significant peaks. The trial structure was refined by three least-squares cycles with isotropic thermal parameters, R=0.091. Three cycles of block diagonal least-squares refinement with anisotropic thermal parameters further reduced R to 0.065. A difference Fourier synthesis was calculated and the positions of fourteen of the twenty-one hydrogen atoms were located. The hydrogen atoms were arbitrarily assigned thermal parameters one unit greater than the atoms to which they were bonded. Three block diagonal least-squares cycles holding the hydrogen atoms constant further refined the model, R=0.055. All shifts were less than one-third of their estimated standard deviations and the structure was considered refined.

Preliminary photographic data and similar cell constants suggested that the Mn(II) complex was isomorphous to the Ni(II) complex. The structure factors calculated for the Mn(II) data using refined isotropic coordinates from the nickel compound differed by a relatively constant factor from those for the Ni(II) data. Therefore, the structures were considered isomorphous. A difference Fourier synthesis revealed no peaks attributable to additional atoms. A Fourier synthesis phased on all atoms was calculated to improve the atomic coordinates. Three cycles of least-squares refinement with individual isotropic thermal paramameters reduced R to 0.13. Three block diagonal least-squares cycles using anisotropic thermal parameters further reduced R to 0.076. A difference Fourier synthesis revealed the positions of all twenty-one hydrogen atoms in the structure. The hydrogen atoms were assigned thermal parameters one unit larger than the refined isotropic parameter of the bonded atoms. Three cycles of block diagonal least-squares refinement holding the hydrogen parameters constant reduced R to 0.062. Less than 3% of the shifts were larger than one-third of their respective standard deviations and the structure was considered refined.

Results for $[M(DAPSC)(H_2O)_2](NO_3)_2 \cdot H_2O$ (M=Mn,Ni)

The final positional and thermal parameters for the non-hydrogen atoms are listed in Table 23. Probable positional parameters and bond distances for the hydrogen atoms are in Table 24. Intramolecular bond distances and angles and short intermolecular contacts are given in Table 25. Least-squares planes and deviations appear in Table 26. The observed and calculated structure factors are in Table 27. Figure 10 is an ORTEP[58] drawing of the complex ion illustrating the numbering scheme. An ORTEP[58] packing diagram of the unit cell contents projected down the a axis is shown in Figure 11.

Structure Solution and Refinement for $[Cu(DAPSC)(H_2O)_2](NO_3)_2 \cdot H_2O$

The Y-coordinate of the copper atom was established from a three-dimensional sharpened Patterson function. Assuming space group P_c, the X and Z coordinates were set at an arbitrary value of ½. Fourier syntheses phased on the copper and subsequently located atoms indicated that the molecule

Table 23

FINAL POSITIONAL AND THERMAL PARAMETERS (x 10^4) FOR THE NON-HYDROGEN ATOMS OF $[M(DAPSC)(H_2O)_2](NO_3)_2 \cdot H_2O$ (M = Mn, Ni) WITH THEIR RESPECTIVE ESTIMATED STANDARD DEVIATIONS IN PARENTHESES

The coordinates of each atom are listed in the order of the metal atoms

ATOM	X	Y	Z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Mn	818(1)	1084(1)	2479(1)	95(1)	29(1)	53(1)	-4(2)	68(2)	1(1)
Ni	800(1)	1254(1)	2430(1)	63(1)	30(1)	48(1)	-3(2)	39(1)	4(1)
O1	896(5)	-387(3)	2251(4)	101(7)	17(2)	49(5)	4(7)	80(9)	-7(5)
	865(6)	-404(4)	2332(5)	106(6)	40(3)	58(5)	3(8)	78(8)	-12(7)
O2	262(5)	731(3)	3991(4)	95(6)	17(2)	38(4)	-2(6)	69(8)	6(5)
	282(5)	736(3)	3946(4)	97(6)	29(3)	53(4)	3(7)	65(9)	-4(6)
O3	2706(5)	1108(4)	3494(5)	78(6)	44(3)	62(5)	6(8)	47(9)	-11(7)
	2552(5)	1161(4)	3371(5)	88(6)	62(4)	66(5)	-1(8)	52(9)	-10(8)
O4	-1170(5)	1004(4)	1554(4)	84(6)	30(3)	52(4)	-3(7)	58(9)	-6(6)
	-1019(5)	1108(4)	1583(4)	66(5)	44(3)	54(4)	-4(7)	45(8)	-4(6)
N1	1094(6)	2352(4)	1543(5)	65(7)	17(3)	40(5)	-7(7)	50(9)	13(6)
	1087(6)	2356(4)	1512(5)	75(7)	27(3)	53(6)	-12(8)	57(10)	4(7)
N2	1360(6)	760(4)	856(5)	69(7)	25(3)	35(5)	-11(7)	40(10)	-8(6)
	1318(6)	745(4)	905(5)	71(7)	34(3)	45(5)	-2(8)	49(10)	-5(7)
N3	1486(6)	-136(4)	658(5)	73(7)	21(3)	29(5)	3(7)	44(10)	-7(6)
	1443(6)	-151(4)	704(5)	83(7)	27(3)	51(5)	-2(8)	55(10)	-7(7)
N4	1270(7)	-1586(4)	1245(5)	92(8)	20(3)	47(5)	-1(8)	33(11)	-2(7)
	1239(6)	-1599(4)	1316(6)	86(8)	36(4)	76(6)	-7(8)	52(12)	-8(8)
N5	463(6)	2352(4)	3383(5)	72(7)	18(3)	44(5)	2(7)	62(10)	0(6)

Table 23 - continued

ATOM	X	Y	Z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
	478(6)	2369(4)	3376(5)	74(7)	23(3)	46(5)	-9(8)	45(10)	5(7)
N6	118(6)	2212(4)	4336(5)	90(8)	20(3)	35(5)	1(8)	69(10)	-5(6)
	149(6)	2210(4)	4356(6)	102(8)	23(3)	61(6)	-1(8)	82(11)	-2(7)
N7	-257(7)	1157(4)	5546(5)	113(8)	26(3)	45(5)	4(9)	104(11)	1(7)
	-228(6)	1132(4)	5556(5)	131(8)	32(4)	52(5)	-6(9)	101(11)	-1(8)
C1	1420(7)	2294(5)	575(6)	64(9)	30(4)	39(6)	-13(10)	44(13)	18(8)
	1426(7)	2268(5)	548(6)	67(8)	38(4)	38(6)	-1(10)	41(12)	24(9)
C2	1604(8)	3045(6)	-20(7)	90(10)	33(4)	40(6)	-9(11)	57(13)	19(9)
	1605(8)	3014(6)	-71(7)	101(10)	41(5)	63(8)	-6(11)	70(15)	14(10)
C3	1418(9)	3874(6)	416(7)	112(10)	30(4)	45(6)	0(12)	54(14)	30(10)
	1467(8)	3869(6)	361(7)	105(10)	46(5)	72(8)	-23(13)	64(14)	30(11)
C4	1090(8)	3946(6)	1413(7)	105(10)	22(4)	57(7)	-22(12)	52(14)	2(10)
	1131(8)	3951(5)	1353(7)	110(10)	29(5)	78(8)	-16(11)	80(15)	16(9)
C5	937(7)	3153(5)	1960(6)	62(9)	15(4)	47(6)	-2(9)	35(12)	15(8)
	957(7)	3166(5)	1930(7)	69(8)	27(4)	52(6)	-1(9)	34(12)	8(8)
C6	1604(7)	1367(5)	221(6)	62(8)	32(4)	28(6)	-2(9)	43(12)	8(7)
	1590(7)	1329(5)	218(6)	68(18)	33(4)	54(6)	-12(10)	53(12)	2(9)
C7	2051(9)	1210(6)	-804(8)	110(11)	43(5)	62(8)	-24(13)	100(15)	-24(10)
	2048(9)	1098(6)	-809(7)	149(12)	54(6)	62(8)	0(14)	139(16)	8(11)
C8	1194(7)	-682(5)	1450(6)	54(8)	21(4)	37(6)	-2(9)	21(11)	-12(8)
	1151(7)	-712(5)	1514(6)	65(8)	39(4)	45(6)	2(10)	49(12)	-14(9)
C9	602(8)	3144(5)	3034(7)	64(9)	18(4)	48(6)	-14(9)	35(12)	1(8)

Table 23 - continued

ATOM	X	Y	Z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
	617(7)	3175(5)	3026(7)	75(9)	30(4)	66(7)	-4(10)	70(13)	-7(9)
C10	453(8)	3982(5)	3651(7)	100(10)	20(4)	70(7)	5(11)	89(14)	12(10)
	447(9)	4004(5)	3642(8)	145(12)	24(4)	87(9)	-18(11)	119(17)	-12(10)
C11	61(7)	1324(5)	4626(6)	55(8)	24(4)	38(6)	3(9)	31(11)	1(8)
	87(7)	1313(6)	4607(6)	73(8)	30(4)	51(6)	11(10)	65(11)	0(9)
N8	2889(7)	1808(5)	6153(6)	86(9)	51(4)	47(6)	-35(10)	34(12)	7(8)
	2926(7)	1746(5)	6127(6)	112(9)	55(4)	57(6)	-20(10)	46(12)	-8(9)
O5	3024(7)	2407(5)	5529(6)	172(10)	55(4)	63(6)	-62(11)	65(13)	23(8)
	3053(7)	2367(5)	5496(6)	160(9)	67(4)	78(6)	-51(10)	53(12)	36(8)
O6	2898(7)	1029(5)	5819(6)	145(9)	42(4)	97(7)	-14(10)	63(13)	-6(9)
	2860(7)	970(4)	5774(6)	152(9)	49(4)	129(8)	-16(9)	81(14)	-12(9)
O7	2742(7)	1982(5)	7053(6)	162(10)	85(5)	66(6)	-48(12)	94(13)	-18(9)
	2842(7)	1923(6)	7069(6)	169(10)	112(6)	73(6)	-44(12)	82(13)	-25(10)
N9	4702(7)	1631(4)	1902(5)	85(8)	25(3)	47(5)	13(8)	59(11)	4(7)
	4714(7)	1609(5)	1883(6)	94(8)	40(4)	59(6)	1(9)	54(11)	7(7)
O8	5202(8)	1467(5)	1159(6)	207(11)	44(4)	101(7)	51(10)	199(15)	27(8)
	5363(7)	1452(5)	1234(6)	172(9)	70(5)	117(7)	74(10)	180(14)	42(9)
O9	4156(6)	2342(4)	1874(6)	135(8)	37(3)	88(6)	42(9)	139(12)	34(7)
	4100(6)	2287(4)	1771(6)	136(8)	50(4)	114(7)	47(9)	134(13)	25(8)
O10	4747(6)	1080(4)	2652(5)	128(7)	37(3)	63(5)	28(9)	84(10)	27(7)
	4692(6)	1062(4)	2648(5)	156(8)	44(4)	82(6)	38(8)	107(12)	29(7)
O11	2366(7)	4578(5)	7782(7)	104(8)	71(5)	133(8)	-29(10)	117(14)	-69(10)
	2462(6)	4503(5)	7773(6)	111(8)	71(4)	123(7)	-2(10)	118(13)	-16(10)

Table 24
POSITIONAL AND THERMAL PARAMETERS (x 10^3) FOR THE HYDROGEN ATOMS OF $[M(DAPSC)(H_2O)_2](NO_3)_2 \cdot H_2O$

ATOM	BONDED TO	DISTANCE,Å	X	Y	Z	B(Å^2)
H1 (M=Ni)	N4	0.98	67	-192	165	4.8
H3	N3	1.01	135	-49	-4	3.8
H4	N7	0.95	-44	60	590	4.5
H5	N7	0.88	-13	161	601	4.5
H6	N6	1.11	-15	263	500	4.2
H7	C7	0.75	170	74	-16	5.5
H8	C7	0.90	173	156	-127	5.5
H11	C10	0.94	78	453	340	5.2
H13	C2	0.99	206	293	-66	4.5
H14	C3	1.21	189	442	-16	5.3
H15	C4	1.07	112	464	160	5.0
H16	O3	1.01	321	113	295	5.4
H19	O4	0.89	-148	104	206	4.3
H20	O11	0.96	227	484	708	6.6
H1 (M=Mn)	N4	0.99	148	-183	202	3.8
H2	N4	0.58	103	-126	104	3.8
H3	N3	1.06	121	-33	-21	3.1
H4	N7	0.91	-9	65	598	3.8
H5	N7	1.14	-72	174	587	3.8
H6	N6	1.03	37	265	501	3.5
H7	C7	0.81	139	109	-122	5.1

Table 24 - continued

ATOM	BONDED TO	DISTANCE, Å	X	Y	Z	B(Å^2)
H8	C7	0.91	245	68	-73	5.1
H9	C7	1.12	291	161	-63	5.1
H10	C10	1.02	64	450	318	4.1
H11	C10	0.92	-37	402	355	4.1
H12	C10	0.96	97	388	439	4.1
H13	C2	0.98	193	300	-68	3.9
H14	C3	1.12	119	445	-19	4.4
H15	C4	1.03	103	455	180	4.3
H16	O3	1.02	187	113	293	4.7
H17	O3	0.81	318	85	323	4.7
H18	O4	0.84	-170	81	185	4.1
H19	O4	0.70	-135	145	143	4.1
H20	O11	0.86	227	466	707	6.5
H21	O11	1.04	146	442	742	6.5

Table 25

INTRAMOLECULAR BOND DISTANCES AND ANGLES AND SHORT INTERMOLECULAR CONTACTS FOR $[M(DAPSC)(H_2O)_2](NO_3)_2 \cdot H_2O$ WITH THEIR ESTIMATED STANDARD DEVIATIONS IN PARENTHESES

(a) Bond Distances (Å)

BOND	M=Mn	Ni	Bond	M=Mn	Ni
M-O3	2.195(6)	2.048(6)	N6-C11	1.383(10)	1.378(10)
M-O4	2.266(6)	2.090(6)	N7-C11	1.309(10)	1.322(10)
M-O1	2.224(5)	2.478(5)	C1-C2	1.390(12)	1.388(12)
M-O2	2.195(5)	2.216(6)	C1-C6	1.487(11)	1.481(11)
M-N1	2.288(6)	2.060(6)	C2-C3	1.392(12)	1.404(13)
M-N2	2.306(7)	2.222(6)	C3-C4	1.386(12)	1.363(13)
M-N5	2.293(6)	2.108(6)	C4-C5	1.400(12)	1.405(11)
O1-C8	1.214(10)	1.214(10)	C5-C9	1.478(11)	1.481(12)
O2-C11	1.246(9)	1.237(9)	C6-C7	1.507(12)	1.515(12)
N1-C1	1.348(10)	1.333(10)	C9-C10	1.502(11)	1.483(12)
N1-C5	1.337(10)	1.335(10)	N8-O5	1.220(10)	1.235(10)
N2-N3	1.377(9)	1.373(9)	N8-O6	1.238(10)	1.230(10)
N2-C6	1.280(10)	1.299(10)	N8-O7	1.198(10)	1.203(10)
N3-C8	1.383(10)	1.396(10)	N9-O8	1.231(11)	1.240(10)
N4-C8	1.384(10)	1.353(10)	N9-O9	1.230(9)	1.220(10)
N5-N6	1.356(9)	1.360(9)	N9-O10	1.233(9)	1.242(9)
N5-C9	1.285(10)	1.299(10)			

(b) Bond Angles (°)

O3-M-O4	175.2(2)	169.3(2)	M-N5-C9	123.1(5)	119.8(5)
O3-M-O1	91.2(2)	85.5(2)	N6-N5-C9	121.6(7)	122.3(7)
O3-M-O2	89.2(2)	87.0(2)	N5-N6-C11	114.7(6)	113.9(6)
O3-M-N1	91.5(2)	94.9(3)	N1-C1-C2	122.4(7)	121.0(7)
O3-M-N2	92.6(2)	90.4(2)	N1-C1-C6	114.6(7)	114.7(7)
O3-M-N5	89.2(2)	92.0(2)	C2-C1-C6	123.0(7)	124.3(7)
O4-M-O1	87.3(2)	84.9(2)	C1-C2-C3	117.1(8)	118.6(8)
O4-M-O2	86.1(2)	85.7(2)	C2-C3-C4	121.3(8)	119.8(8)
O4-M-N1	92.7(2)	95.5(2)	C3-C4-C5	117.6(8)	118.4(8)
O4-M-N2	91.2(2)	90.1(2)	N1-C5-C4	121.7(7)	121.3(7)

Table 25 - continued

(b) continued

O4-M-N5	90.2(2)	93.3(2)	N1-C5-C9	115.7(7)	115.6(7)
O1-M-O2	84.3(2)	73.2(2)	C4-C5-C9	122.6(7)	123.1(7)
O1-M-N1	137.8(2)	139.4(2)	N2-C6-C1	114.2(7)	113.1(7)
O1-M-N2	69.6(2)	66.4(2)	N2-C6-C7	125.8(8)	124.7(7)
O1-M-N5	154.0(2)	145.6(2)	C1-C6-C7	120.0(7)	122.2(7)
O2-M-N1	137.8(2)	147.5(2)	O1-C8-N3	122.5(7)	121.0(7)
O2-M-N2	153.9(2)	139.6(2)	O1-C8-N4	123.4(7)	124.3(8)
O2-M-N5	69.8(2)	72.5(2)	N3-C8-N4	114.1(7)	114.7(7)
N1-M-N2	68.2(2)	72.9(2)	N5-C9-C5	113.3(7)	111.7(7)
N1-M-N5	68.1(2)	75.0(3)	N5-C9-C10	124.0(7)	124.2(8)
N2-M-N5	136.3(2)	147.9(2)	C5-C9-C10	122.7(7)	124.1(7)
M-O1-C8	119.5(5)	115.8(5)	O2-C11-N6	119.5(7)	120.2(7)
M-O2-C11	120.7(5)	115.5(5)	O2-C11-N7	123.6(7)	124.2(7)
M-N1-C1	120.3(5)	121.4(5)	N6-C11-N7	116.9(7)	115.6(7)
M-N1-C5	119.8(5)	117.8(5)	O5-N8-O6	117.9(8)	119.7(8)
C1-N1-C5	119.9(7)	120.7(7)	O5-N8-O7	120.1(8)	118.5(8)
M-N2-N3	115.1(5)	123.0(5)	O6-N8-O7	122.0(8)	121.8(8)
M-N2-C6	122.6(5)	117.8(5)	O8-N9-O9	119.2(7)	120.7(7)
N3-N2-C6	122.1(7)	119.0(6)	O8-N9-O10	119.6(7)	118.9(7)
N2-N3-C8	113.1(6)	113.7(6)	O9-N9-O10	121.2(7)	120.3(7)
M-N5-N6	115.3(5)	117.9(5)			

(c) Short Intermolecular Contacts (Å)

ATOM A	EQUIV.POS.	ATOM B	EQUIV.POS.	DISTANCE	
				M=Mn	Ni
O3	X,Y,Z	O6	X,Y,Z	2.826(9)	2.864(9)
O3	X,Y,Z	O10	X,Y,Z	2.808(9)	2.820(9)
O5	X,Y,Z	O4	½+X,½-Y,½+Z	2.737(9)	2.706(9)
O11	X,Y,Z	O4	½+Y,½-Y,½+Z	2.694(10)	2.697(9)
N7	1+X,Y,Z	O1	1-X,-Y,1-Z	3.218(9)	3.047(9)
N7	1+X,Y,Z	O2	1-X,-Y,1-Z	2.883(8)	2.856(8)
O5	X,Y,Z	N4	½-X,½+Y,½-Z	2.947(10)	2.969(10)
O9	X,Y,Z	N4	½-X,½+Y,½-Z	2.971(9)	2.964(10)
O8	X,Y,Z	N6	½+X,½-Y,Z-½	2.979(10)	2.994(10)
O9	X,Y,Z	N7	½+X,½-Y,Z-½	2.965(9)	2.988(10)

Table 26
LEAST-SQUARES PLANES AND DEVIATIONS FOR $[M(DAPSC)(H_2O)_2](NO_3)_2 \cdot H_2O$ (M=Mn,Ni)

The titles of the planes are given followed by the deviations (x 10^3 Å) of the atoms listed in the left-hand column. Asterisks denote deviations of atoms used to define the plane. The equation of the plane is of the form ax+by+cz=d, where d is the distance (Å) from the origin. The dihedral angles are in degrees and decimal fractions.

Plane 1. Plane Through the Pentagonal Donor Set

Plane 2. Plane Through the Pyridine Ring

	Plane 1		Plane 2	
	M=Mn	Ni	M=Mn	Ni
M	27	1	-8	-3
O3	2221	2042		
O4	-2235	-2078		
O1	4*	9*	-54	14
O2	-6*	-14*	-71	-25
N1	-4*	-7*	-4*	-10*
N2	-1*	-2*	-18	6
N5	7*	13*	-21	-2
C1			-2*	11*
C2			7*	-8*
C3			-7*	4*
C4			1*	-3*
C5			4*	6*
a	0.8519	0.8587	0.8573	0.8612
b	0.0096	0.0092	0.0213	0.0062
c	0.5236	0.5123	0.5144	0.5082
d	1.6348	1.6145	1.6628	1.6011

Plane 3. Plane Through Nitrate Anion 1

Plane 4. Plane Through Nitrate Anion 2

Table 26 - continued

	Plane 3		Plane 4	
	M=Mn	Ni	M=Mn	Ni
N8	3*	9*		
05	-1*	-3*		
06	-1*	-3*		
07	-1*	-3*		
N9			3*	2*
08			-1*	-1*
09			-1*	-1*
010			-1*	-1*
a	0.9141	0.9358	0.7165	0.6153
b	-0.0396	-0.0851	0.4293	0.4866
c	0.4036	0.3422	0.5498	0.6202
d	4.0169	3.5827	5.7088	5.5075

Dihedral Angles

Plane A	Plane B	Angle	
		M=Mn	Ni
1	2	0.90	0.30
1	3	8.25	12.01
1	4	25.52	31.72
2	3	7.94	11.68
2	4	25.01	31.99
3	4	30.70	41.70

Table 27
OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $[M(DAPSC)(H_2O)_2](NO_3)_2 \cdot H_2O$ (M=Mn,Ni)

The structure factors for the reflection (HKL) are listed to the right of the appropriate L value under the corresponding H and K values. FO and FC refer to F_{obs} and F_{calc} respectively. The structure factors for the Mn compound are listed first.

```
   L    FO     FC

H=    0,  K=    0

   2  1050  -1108
   4   102     25
   6   709   -782
   8   174    162
  10   550   -530
  12   190    180

H=    1,  K=    0

   1   867   -901
   3   142    275
   5   223    178
   7   -73    102
   9   240   -227
  11   -71     -6
 -13   367    357
 -11   525   -515
  -9   641    614
  -7   155     94
  -5   248    207
  -3   179   -224
  -1  1153   1128

H=    2,  K=    0

   0  1081   1139
   2  1216  -1134
   4   -54     41
   6   235   -223
   8   153    156
  10   335   -357
  12   222    239
 -12   102   -120
 -10   -72     23
  -8   259    265
  -6   254   -272
  -4   527    503
  -2   550   -575

H=    3,  K=    0

   1  5579  -6034
   3   824    832
   5   594   -612
   7   436    458
   9   -73     58
  11   175    181
 -13   119    113
 -11   221   -218
  -9   448    432
  -7   309   -347
  -5  1730   1708
  -3   -54    -80
  -1   197     39

H=    4,  K=    0

   0   291   -336
   2   305    337
   4   155   -168
   6   -69    -90
   8   -74     33
  10   -75     66
 -12   307   -382
 -10   653    650
  -8   828   -805
  -6   395   -332
  -4   139   -135
  -2    95    -17

H=    5,  K=    0

   1   921   -953
   3   936    918
   5   -70     60
   7   -76     -5
   9   103    -13
```

```
   L    FO     FC

 -13   119    144
 -11   -71    -36
  -9   288    306
  -7   343   -339
  -5   -58     16
  -3   416   -432
  -1   191    173

H=    6,  K=    0

   0   415   -430
   2  2259   2277
   4   -71    -13
   6   200    153
   8   290   -283
 -12   218   -193
 -10   435    440
  -8   352   -528
  -6   224   -196
  -4   837   -858
  -2   471    446

H=    7,  K=    0

   1   168    153
   3   -74    -37
   5   -77      9
   7   -76    -36
 -11   214    234
  -9   439   -444
  -7   616    615
  -5   215    231
  -3   160    175
  -1   106   -101

H=    8,  K=    0

   0   202    219
   2   301    302
   4   505   -510
   6   -75     32
 -12   130    -58
 -10   -71    -72
  -8   286   -291
  -6   307    310
  -4   103    -77
  -2   215    246

H=    9,  K=    0

   1   245    248
   3   968  -1021
   5   -76     46
 -11   -74    -47
  -9   313   -312
  -7   493    490
  -5   -76    -70
  -3   217    221
  -1   -76    -17

H=   10,  K=    0

   0   132     96
   2   145   -138
   4   -81     30
 -10   166   -130
  -8   259    224
  -6   342   -350
  -4   -78    -29
  -2   170   -166

H=   11,  K=    0

   1   -79    -82
  -9   -77     27
  -7   167    159
  -5   -76    -46
  -3   -76    -17
  -1   203   -199
```

```
   L    FO     FC

H=   12,  K=    0

  -6   232   -233
  -4   197    163
  -2   191   -183

H=    0,  K=    1

   1   116    114
   2   802   -734
   3   492   -455
   4   -55     15
   5    97    -75
   6   455   -430
   7    88     76
   8   -65    -54
   9   -70    -16
  10   -73     31
  11   -71      0
  12   -73    -74

H=    1,  K=    1

   0  1164   1194
   1   794   -847
   2   252   -271
   3   890   -807
   4   143    155
   5   640   -625
   6   916   -899
   7   -62     10
   8   534    534
   9   243   -208
  10   373   -346
  11   168    141
  12   179    199
 -13   -74     50
 -12   217    215
 -11   416   -418
 -10   246   -245
  -9   324    341
  -8   150   -115
  -7   -60     37
  -6   493   -497
  -5   -54    129
  -4   600    635
  -3   540   -551
  -2   415    273
  -1  1035    990

H=    2,  K=    1

   0   876   -912
   1   872   -912
   2   332    353
   3   625   -530
   4   180   -213
   5   603   -601
   6   383    365
   7   677    680
   8   220   -225
   9   -73    -75
  10   205    194
  11   130    119
  12   158   -174
 -13   178    157
 -12   207   -206
 -11   282   -262
 -10   160    140
  -9   349    353
  -8   240   -228
  -7   557   -571
  -6   150    -34
  -5  1457   1392
  -4  1067  -1106
  -3  1050  -1024
  -2   479   -406
  -1   803    827

H=    3,  K=    1
```

```
   L    FO     FC

   0   280   -294
   1   -55    -16
   2   261    245
   3   234    255
   4   205    222
   5   -60     29
   6   -64    -24
   7   200    232
   8   -73      1
   9   -75     59
  10   -72      0
  11   -76     28
 -13   -74    101
 -12   193   -193
 -11   -71    -81
 -10   -71     42
  -9   -67     92
  -8   -55    -39
  -7   107     90
  -6   -56    -38
  -5   595   -660
  -4   145     80
  -3    82     64
  -2   369    404
  -1   675   -795

H=    4,  K=    1

   0   903   -896
   1  1126  -1073
   2   955    910
   3   702    687
   4   115    107
   5   194   -201
   6   351    353
   7   411    411
   8   -75     50
   9   208   -210
  10   -75     53
 -13   -73     -7
 -12   -71     80
 -11   -72   -112
 -10   442    452
  -9   544    339
  -8   522   -627
  -7   179   -216
  -6   -57     89
  -5   591    564
  -4   248    192
  -3   -54    -57
  -2   -55    104
  -1   647   -574

H=    5,  K=    1

   0   968   -941
   1   951    933
   2  1026   1009
   3   472   -472
   4   137    151
   5   -69     38
   6   145    142
   7   -75    -62
   8   264   -257
   9   107     88
  10   103     94
 -13   129    -79
 -12   196   -210
 -11   303    304
 -10   420    419
  -9   247   -271
  -8   560   -573
  -7   395    387
  -6   585    599
  -5   110     25
  -4  1000   -942
  -3   623    672
  -2   676    677
  -1   157    154
```

```
     L      FO      FC

 H=     6,  K=       1

     0     240     249
     1     -64      37
     2     192     188
     3     135    -110
     4     -72      14
     5     -74     -85
     6     -77     -37
     7     -75      25
     8     -76    -120
     9     123     -51
   -12     -73     -70
   -11     200     204
   -10     -73      35
    -9     -72     -60
    -8     109    -116
    -7     102     112
    -6     182    -158
    -5      87     -30
    -4     476     475
    -3      66       1
    -2     -61      21
    -1     -61     -23

 H=     7,  K=       1

     0     232     214
     1     427     433
     2     415     418
     3     476    -462
     4     314    -315
     5     118      -2
     6     142     161
     7     246    -251
     8     267    -247
   -12     136    -121
   -11     -71     -23
   -10     -71      71
    -9     238    -237
    -8     -73     -72
    -7     380     369
    -6     193     194
    -5     -67    -129
    -4     750    -760
    -3     155     192
    -2     356     415
    -1     245    -280

 H=     8,  K=       1

     0     146    -158
     1     273     269
     2     367    -386
     3     463    -471
     4     279     269
     5     -77      40
     6     109     -99
     7     -79     -91
   -12     -77     113
   -11     185     192
   -10     288    -301
    -9     325    -328
    -8     191     185
    -7     452     466
    -6     298    -305
    -5     522    -523
    -4     162     148
    -3     621     637
    -2     356    -368
    -1     263    -260

 H=     9,  K=       1

     0     -77      -3
     1     -78     -16
     2     -78      22
     3     166    -198
     4     -77     -44
```

```
     L      FO      FC

     5     -78     -16
     6     -81      48
   -11     -75       9
   -10     161    -183
    -9     -72       9
    -8     -74      26
    -7     119     126
    -6     -75      60
    -5     -76      31
    -4     109     -85
    -3     123    -137
    -2     -76      21
    -1     -77     -13

 H=    10,  K=       1

     0     222     219
     1     -77      24
     2     247    -258
     3     235    -229
     4     242     243
   -10     -78    -105
    -9     234    -210
    -8     224     249
    -7     118     110
    -6     135    -175
    -5     -77     -60
    -4     126    -102
    -3     298     283
    -2     -79     -87
    -1     252    -244

 H=    11,  K=       1

     0     -80     145
     1     -79      28
     2     -81     -31
    -9     274     250
    -8     223     225
    -7     -76     -77
    -6     190    -200
    -5     -78      78
    -4     156     171
    -3     -77     -24
    -2     269    -280
    -1     156     183

 H=    12,  K=       1

    -6     -80     -43
    -5     -80     -40
    -4     -81      12
    -3     -81     105
    -2     -81       8
    -1     -82     -74

 H=     0,  K=       2

     0     825    -673
     1    1067   -1056
     2     387    -397
     3    1369    1400
     4     259     251
     5     613    -630
     6     779    -738
     7     497     475
     8     456     439
     9     501    -508
    10     131    -117
    11     355     342
    12     179     120

 H=     1,  K=       2

     0     811    -764
     1     276     286
     2     722     630
     3     867    -753
     4     -54     -94
     5     -56     -29
```

```
     L      FO      FC

     6     424     433
     7     -63     -64
     8     120    -161
     9     -73    -132
    10     -72      66
    11     -71       3
    12     -75     -55
   -12     402    -400
   -11     -59     -24
   -10     -71      28
    -9     -63     -82
    -8     -64      -8
    -7     477    -460
    -6     870     884
    -5     745     701
    -4     275    -297
    -3     119    -116
    -2     604    -490
    -1     324     351

 H=     2,  K=       2

     0     243    -195
     1     811    -756
     2     -57    -122
     3     460    -434
     4     154     162
     5     392    -390
     6     495    -475
     7     751     763
     8     350     366
     9     -73    -101
    10     -72      44
    11     -73     -13
    12     -77      -2
   -13     201     191
   -12     -73    -127
   -11     129    -135
   -10     -70     -26
    -9     -67     -59
    -8      93     129
    -7     269    -269
    -6     121      97
    -5    1044    1044
    -4      91      84
    -3     479    -495
    -2     710     632
    -1    1020    1019

 H=     3,  K=       2

     0     684     538
     1     653     584
     2     648     691
     3     230     259
     4    1150   -1123
     5     200    -176
     6     642     640
     7     434     439
     8     195    -186
     9     186    -170
    10     103      91
    11     116      30
   -13     -72      26
   -12     596    -617
   -11     -73    -125
   -10     331     323
    -9     119     120
    -8     571    -601
    -7     677    -662
    -6     976     961
    -5    1051     967
    -4    1503   -1460
    -3     274    -297
    -2     832     879
    -1     144     145

 H=     4,  K=       2

     0     200    -237
```

```
     L      FO      FC

     1     157     161
     2     -57     -12
     3     367    -373
     4     347     327
     5     179     159
     6     -59      21
     7     145    -137
     8     -75      75
     9     -72     -51
    10     120      64
   -13     172    -183
   -12     108     -38
   -11     450     475
   -10     113      75
    -9     -69     -45
    -8     -65      52
    -7     -61      61
    -6     480     459
    -5     615    -597
    -4     531    -563
    -3     114     -51
    -2     129    -130
    -1     652     601

 H=     5,  K=       2

     0     730    -751
     1     -60     -51
     2     531     654
     3     -63      79
     4     135     158
     5     -70     -43
     6     108     116
     7     157     163
     8     237    -296
     9     163    -200
    10     124      72
   -13     -73      43
   -12     344    -358
   -11     135     117
   -10     389     399
    -9     -59      59
    -8     132    -108
    -7     176    -177
    -6     224     198
    -5      89    -110
    -4     575    -578
    -3     -57      37
    -2     212     220
    -1     276    -263

 H=     6,  K=       2

     0     142    -157
     1     224    -222
     2     216    -216
     3     105    -101
     4     -73     -70
     5     277     240
     6     -76      25
     7     357    -357
     8     194    -199
     9     208     175
   -12     -72     -75
   -11     775     801
   -10     162     136
    -9     453    -434
    -8     103     -40
    -7     214     213
    -6     424     414
    -5     217    -252
    -4     656    -641
    -3    1075    1088
    -2     243     239
    -1     819    -821

 H=     7,  K=       2

     0     177    -212
     1     -69      56
   L    FO     FC       L    FO     FC       L    FO     FC       L    FO     FC

   2   -72      2                           11   152   -107       8   125    142
   3   -74    -36    H=  11,  K=   2       -13   -75    -39       9   206    219
   4   -77     78                          -12   302   -299      10   122   -109
   5   157   -112       0   -80     53     -11   140   -114     -12   -73     50
   6   114   -120       1   -79    -17     -10   -72   -114     -11   467    459
   7   121    -43       2   -80     -2      -9   532   -526     -10   120    126
   8   150    127      -8   160    152      -8   123   -145      -9   -71    -26
 -12   116    104      -7   -78    -84      -7   180    187      -8   560    557
 -11   -73     38      -6   -77    -25      -6  1061   1050      -7   239    248
 -10   317   -313      -5   -76    -29      -5   -54    -95      -6   250   -251
  -9   -73   -125      -4   -76     72      -4   679   -725      -5   557   -651
  -8   -74    -39      -3   -78     50      -3   533    618      -4    97    -94
  -7   104    -85      -2   173   -161      -2   614    642      -3   432    444
  -6   109   -103      -1   -76    -20      -1   113   -168      -2   282   -302
  -5   307   -238                                                 -1   776   -779
  -4   272    292    H=  12,  K=   2       H=   3,  K=   3
  -3   272    254                                                H=   6,  K=   3
  -2   -65    -38      -6   -79      3       0   -55    -56
  -1   -67    113      -5   233    214       1   293    307       0   149   -147
                       -4   -81     68       2   600   -642       1   -65    112
H=   8,  K=   2        -3   149   -158       3   434   -436       2   163   -155
                       -2   -82   -134       4   257   -253       3   305    353
   0   146    134      -1   246    233       5   308    311       4   185    204
   1   -75     82                            6   -66     18       5   -75     58
   2   -76    -20    H=   0,  K=   3         7   -70     -5       6   -77    -92
   3   238   -221                            8   170    175       7   -75    -50
   4   -77    -24       1   452    430       9   -73      2       8   -76    -69
   5   -75      0       2   602    563      10   -73     63       9   -77    -39
   6   -77     16       3   557    496      11   -75    -77     -12   -75     84
   7   132   -106       4   507   -549     -13   -75    -68     -11   -71     14
 -11   261    271       5   151    125     -12   -72    -83     -10   -71    -48
 -10   106   -112       6   119    107     -11   -71     42      -9   190   -200
  -9   247   -263       7   303   -292     -10   224    222      -8   -72   -113
  -8   106     55       8   123   -122      -9   123    135      -7   -56    -93
  -7   133    155       9   -71    -95      -8   101    152      -6   115    102
  -6   -73    127      10   160    165      -7   196   -190      -5   -64   -115
  -5   273   -269      11   127   -115      -6   228    208      -4   -62      9
  -4   -72    -32      12   -73    -37      -5   -56     75      -3   -62     31
  -3   300    304                           -4   121    -97      -2   537    541
  -2   -71    -18    H=   1,  K=   3        -3   504   -480      -1   142     86
  -1   -73     59                           -2   483   -462
                        0   536    435      -1   218    197    H=   7,  K=   3
H=   9,  K=   2         1   328   -324
                        2   384   -231    H=   4,  K=   3         0   -70   -104
   0   271    249       3   295   -210                            1   107     54
   1   111     70       4   208   -255       0   215   -234       2   -72    -29
   2   -73    -14       5   209   -213       1   -56      8       3   -76   -127
   3   -77     30       6   123    153       2   564    562       4   -77      6
   4   156    165       7   768    770       3   -60    -16       5   157    130
   5   -79     51       8   250   -229       4   227   -232       6   -75    -75
   6   139    -77       9   320   -328       5   -67    120       7   277   -264
 -11   -75     61      10   472    455       6   244    251       8   -79     58
 -10   499   -502      11   -73      2       7   -72    -73     -12   185    187
  -9   109   -103      12   -75     40       8   351   -339     -11   366    331
  -8   414    404     -12   274   -289       9   131    107     -10   -74   -173
  -7   -75     31     -11   -70      1      10   176    187      -9   163    203
  -6   354   -349     -10   273    266     -13   127   -104      -8   193    200
  -5   196   -184      -9   203    192     -12   333   -334      -7   218    216
  -4   112    107      -8   170   -160     -11   195    246      -6   420   -420
  -3   292    232      -7   139   -135     -10   -71   -100      -5   546   -554
  -2   343   -344      -6   318    341      -9   411   -405      -4   512    507
  -1   -78    -74      -5   -55    196      -8   439   -450      -3   557    554
                       -4   215   -222      -7   463    472      -2   159   -148
H=  10,  K=   2        -3   986   -989      -6   444    462      -1   397   -403
                       -2   499   -424      -5   359   -361
   0   -77    -32      -1   420    450      -4   -55    -42    H=   8,  K=   3
   1   -76     13                           -3   105    -79
   2   -77    -36    H=   2,  K=   3        -2   240    279       0   250    243
   3   -79     43                           -1   329    323       1   -75    -36
   4   -80     36       0   348   -395                            2   221   -206
 -10   132    -52       1   408   -326    H=   5,  K=   3         3   159    119
  -9   171    169       2   172    -60                            4   194    182
  -8   -76    145       3   662    626       0   287    331       5   -76      2
  -7   -74     53       4   610   -603       1   695    701       6   135   -146
  -6   -74     49       5   200    213       2   215   -209       7   -79     48
  -5   156    150       6   471    503       3   214   -244     -11   113   -101
  -4   -78    119       7   387   -405       4   205   -188     -10   376   -365
  -3   171   -167       8   391   -392       5   157    178      -9   -73   -110
  -2   123    -32       9   160    172       6   148    -44      -8   -73    -12
  -1   -77     55      10   111    143       7   158   -156      -7   322   -330
```

```
    L    FO     FC

   -6   325   -331
   -5   184    195
   -4   690    707
   -3   -72     -6
   -2   305   -311
   -1   113    135

 H=     9,  K=    3

    0   142    -20
    1   -79    111
    2   -78    -91
    3   -76    -16
    4   -79   -108
    5   -79    -56
  -11   -77    -80
  -10   -75     22
   -9   111      9
   -8   -74    126
   -7   192    193
   -6   -75      3
   -5   170   -164
   -4   -77    108
   -3   -75     13
   -2   -77    -30
   -1   -76   -115

 H=    10,  K=    3

    0   287    266
    1   -75    -24
    2   183   -128
    3   -80     46
    4   -80     41
  -10   390   -395
   -9   192    213
   -8   -75     51
   -7   109   -122
   -6   123   -139
   -5   193    173
   -4   213    206
   -3   241   -227
   -2   257   -265
   -1   193    129

 H=    11,  K=    3

    0   112    -89
    1   -80   -111
    2   -80     -4
   -8   -78     24
   -7   -78     65
   -6   147    132
   -5   111    123
   -4   -77    -17
   -3   301   -313
   -2   -78    -22
   -1   234    209

 H=    12,  K=    3

   -5   -81     -4
   -4   -80    109
   -3   -81    -33
   -2   -81    -60

 H=     0,  K=    4

    0  2106  -2009
    1   780   -778
    2   395    465
    3   702    679
    4   -54    -90
    5   195   -221
    6   585    592
    7   524    508
    8   803   -812
    9   -71     31
   10   307    300
   11   107   -125
```

```
    L    FO     FC

   12   133   -112

 H=     1,  K=    4

    0   462    406
    1   584    590
    2   777   -685
    3    81   -134
    4   150    127
    5   -59    162
    6   119    129
    7   249   -249
    8   143   -159
    9   344    335
   10   -71    -22
   11   -72      4
   12   167   -157
  -12   138   -164
  -11   -70    -82
  -10   144   -161
   -9   508   -515
   -8   -67    -84
   -7   -62     37
   -6   293    250
   -5   628   -609
   -4   148   -190
   -3  1000    938
   -2   -54     61
   -1   255   -277

 H=     2,  K=    4

    0   718   -725
    1   561    586
    2   311    323
    3   141   -115
    4   723   -705
    5   165   -217
    6   462    478
    7   254    248
    8   139   -150
    9   -73    -91
   10   319    330
   11   121   -115
  -12   137    -69
  -11   281   -299
  -10   -72      4
   -9   -70    -44
   -8   397   -392
   -7   207   -210
   -6   551    503
   -5   354    326
   -4   576   -567
   -3   249   -239
   -2   458    466
   -1   475   -442

 H=     3,  K=    4

    0   345   -355
    1   689    710
    2   425    411
    3   437   -457
    4   435   -440
    5   521    570
    6   182    210
    7   370   -352
    8   283   -300
    9   284    302
   10   121   -124
   11   -76    -54
  -12   170   -172
  -11   148    158
  -10   272   -271
   -9   230   -237
   -8   -65     13
   -7  1187   1165
   -6   746    753
   -5  1252  -1224
   -4   319   -302
```

```
    L    FO     FC

   -3    77    123
   -2   481    495
   -1   435    514

 H=     4,  K=    4

    0   181   -139
    1   107    -55
    2   205   -184
    3   155    173
    4   132    154
    5   -67    -21
    6   -71   -101
    7   -73     40
    8   108     61
    9   -73     -7
   10   -77   -125
  -12   158    151
  -11   201    192
  -10   -71     35
   -9   205    204
   -8   610    504
   -7   -63    114
   -6   103     37
   -5   283   -267
   -4   385    374
   -3   132    -79
   -2   338   -413
   -1   157    165

 H=     5,  K=    4

    0   -60    -30
    1   612    630
    2   106   -135
    3   235   -513
    4   -69     92
    5   231    286
    6   -75     38
    7   -75   -104
    8   -74    -85
    9   -75     51
  -12   173   -199
  -11   228    243
  -10   367    572
   -9   203   -219
   -8   -69    -58
   -7   375    356
   -6   277    271
   -5   319   -295
   -4   129   -150
   -3   303    290
   -2   159    161
   -1   351   -347

 H=     6,  K=    4

    0   130    146
    1   301    275
    2   172   -203
    3   163   -156
    4   -73    -30
    5   -76     90
    6   232   -244
    7   -75    -52
    8   241    213
    9   200    177
  -12   500    527
  -11   223    235
  -10   345   -301
   -9   312    313
   -8   170    153
   -7   179   -190
   -6   571   -561
   -5   428   -443
   -4   562    544
   -3   221    219
   -2   375   -373
   -1   320   -344
```

```
    L    FO     FC

 H=     7,  K=    4

    0   158   -143
    1   -72     68
    2   -74     65
    3   -75     24
    4   -77    -17
    5   -75    -59
    6   -75    -76
    7   -77     84
    8   -77     -4
  -12   -75    -25
  -11   -72    -41
  -10   176   -176
   -9   -72    -51
   -8   225   -222
   -7   447   -442
   -6   -71    -47
   -5   -59    -43
   -4   218    179
   -3   168   -163
   -2   -68     33
   -1   227    232

 H=     8,  K=    4

    0   -75      7
    1   -76    -11
    2   193   -173
    3   -77     30
    4   141    154
    5   -75      4
    6   153   -181
  -11   150    152
  -10   141   -147
   -9   156   -156
   -8   145    131
   -7   -74    -75
   -6   294   -262
   -5   279   -272
   -4   243    266
   -3   125    151
   -2   -74   -120
   -1   112    -87

 H=     9,  K=    4

    0   -79    107
    1   151   -121
    2   159   -155
    3   227    227
    4   -79    126
    5   -81    -34
  -10   190   -194
   -9   277    269
   -8   164   -197
   -7   250   -257
   -6   130    150
   -5   412    413
   -4   202    206
   -3   -76    -96
   -2   -78    -69
   -1   -78     49

 H=    10,  K=    4

    0   -78   -121
    1   -76     27
    2   -78     13
    3   -79    -23
    4   -79    -51
   -9   158    154
   -8   -75     36
   -7   -75    115
   -6   285    285
   -5   -75      1
   -4   -76    -19
   -3   -78    -53
   -2   -76     57
   -1   -76     14
```

L	FO	FC
H= 11, K= 4		
0	-81	114
1	-80	-40
-8	-79	66
-7	-78	7
-6	137	182
-5	-78	32
-4	-77	50
-3	145	-113
-2	141	-102
-1	156	124
H= 12, K= 4		
-4	292	-234
-3	154	-111
H= 0, K= 5		
1	195	138
2	283	205
3	101	83
4	155	-193
5	111	-47
6	-80	10
7	206	-212
8	171	-157
9	208	-181
10	143	133
11	113	-124
12	-75	34
H= 1, K= 5		
0	617	-846
1	106	-49
2	245	-142
3	459	-298
4	380	-358
5	565	477
6	129	141
7	-58	-31
8	358	-333
9	126	112
10	-71	-34
11	-73	33
-12	297	-297
-11	-71	-38
-10	-71	38
-9	201	-284
-8	-66	-64
-7	136	-129
-6	380	374
-5	273	-258
-4	849	-865
-3	1620	1386
-2	1495	1402
-1	300	244
H= 2, K= 5		
0	219	212
1	303	370
2	352	316
3	746	-753
4	780	722
5	741	743
6	140	-133
7	556	-554
8	-72	-9
9	219	195
10	168	-169
11	-74	0
-12	-73	33
-11	102	103
-10	119	111
-9	173	210
-8	107	101

L	FO	FC
-7	277	250
-6	-59	32
-5	266	-337
-4	500	458
-3	1049	1032
-2	910	-811
-1	-53	-92
H= 3, K= 5		
0	139	145
1	341	-357
2	305	-271
3	-59	-93
4	-62	-23
5	212	215
6	-70	29
7	-72	-31
8	152	105
9	117	87
10	107	110
-12	140	136
-11	-70	18
-10	-71	24
-9	147	129
-8	366	354
-7	183	-155
-6	225	213
-5	130	138
-4	212	172
-3	152	-148
-2	214	-243
-1	353	343
H= 4, K= 5		
0	91	62
1	769	842
2	-60	-49
3	440	-446
4	146	147
5	568	495
6	273	-234
7	142	-63
8	-74	0
9	155	118
10	-77	-88
-12	-74	-99
-11	257	258
-10	185	185
-9	-72	-50
-8	420	433
-7	585	348
-6	-62	14
-5	565	-556
-4	197	218
-3	359	382
-2	1190	-1153
-1	675	-705
H= 5, K= 5		
0	474	454
1	326	-310
2	566	-598
3	-67	18
4	410	402
5	294	-277
6	208	-212
7	-73	-12
8	239	216
9	-76	17
-12	493	509
-11	-70	-20
-10	282	-280
-9	195	-198
-8	-70	38
-7	153	-171
-6	208	-266
-5	-63	56

L	FO	FC
-4	140	154
-3	257	-273
-2	744	-755
-1	559	533
H= 6, K= 5		
0	112	-123
1	-69	-22
2	218	216
3	-73	101
4	-75	-10
5	125	53
6	120	-139
7	-76	-48
8	-75	54
-12	150	-159
-11	-74	-91
-10	-72	69
-9	-72	0
-8	-74	-112
-7	427	-417
-6	-69	18
-5	-67	-94
-4	122	-114
-3	138	-181
-2	-65	30
-1	98	51
H= 7, K= 5		
0	422	428
1	-73	-61
2	274	-285
3	-77	52
4	199	198
5	-76	-66
6	381	-355
7	-60	153
-11	-75	125
-10	259	-259
-9	281	-300
-8	157	-161
-7	314	-312
-6	309	-273
-5	129	148
-4	721	727
-3	275	-281
-2	559	-573
-1	631	632
H= 8, K= 5		
0	208	-215
1	153	-103
2	-77	102
3	258	280
4	-76	-44
5	232	-248
6	-79	111
-11	402	-400
-10	-74	47
-9	193	188
-8	246	243
-7	166	-126
-6	108	97
-5	406	404
-4	122	-85
-3	252	-273
-2	231	223
-1	308	303
H= 9, K= 5		
0	-78	-15
1	-75	9
2	-77	-47
3	-77	-60
4	-79	34
5	-80	7

L	FO	FC
-10	-77	65
-9	152	-118
-8	-74	65
-7	-75	87
-6	179	154
-5	-78	66
-4	-76	135
-3	-78	45
-2	155	115
-1	-79	-11
H= 10, K= 5		
0	234	-289
1	299	-304
2	-79	49
3	158	178
-9	373	359
-8	187	198
-7	-76	24
-6	126	142
-5	162	138
-4	-76	-71
-3	266	-265
-2	181	162
-1	308	292
H= 11, K= 5		
0	201	-176
1	-83	90
-7	155	-141
-6	-77	5
-5	-76	-35
-4	175	-172
-3	-79	-31
-2	176	169
-1	120	-112
H= 0, K= 6		
0	1553	-1469
1	930	903
2	236	320
3	1357	-1316
4	120	52
5	355	362
6	374	357
7	559	-563
8	156	-129
9	413	397
10	533	526
11	-72	-16
H= 1, K= 6		
0	664	630
1	476	452
2	-55	-82
3	86	-90
4	322	330
5	235	-220
6	-66	-78
7	266	-238
8	105	109
9	249	257
10	-71	-26
11	-75	-25
-12	368	370
-11	191	192
-10	107	-28
-9	135	-110
-8	345	346
-7	249	239
-6	585	-506
-5	-59	-14
-4	862	831
-3	408	395
-2	733	-674
-1	373	-381

```
   L    FO    FC

H=    2,  K=   6

   0   444  -417
   1   594   564
   2    90    31
   3   562  -542
   4   126  -131
   5   713   630
   6   144   154
   7   354  -416
   8   314  -294
   9   208   229
  10   129   104
  11   -77    21
 -12   -74   -79
 -11   -72    83
 -10   -71   117
  -9   -72    60
  -8   326  -321
  -7   246   257
  -6   327   306
  -5   328  -358
  -4   -57   -74
  -3   791   741
  -2   518   469
  -1   176  -214

H=    3,  K=   6

   0   119   156
   1   359   348
   2   566  -573
   3    75   -92
   4  1032  1058
   5   -63    66
   6   388  -363
   7   234  -218
   8   185   145
   9   -73    12
  10   123   -92
 -12   262   250
 -11   308   320
 -10   -70    66
  -9   565  -563
  -8   540   520
  -7   306   283
  -6   605  -616
  -5   777  -753
  -4   736   760
  -3    22   -33
  -2  1034 -1012
  -1   174  -198

H=    4,  K=   6

   0   221   223
   1   202  -195
   2   467  -476
   3   -64    52
   4   -68   112
   5   215  -218
   6   226   243
   7   -75    16
   8   -73    41
   9   -74    38
  10   120  -117
 -12   155   151
 -11   433  -430
 -10   160  -144
  -9   -72    24
  -8   107    67
  -7   401  -410
  -6   184  -152
  -5   491   500
  -4   210  -147
  -3   509  -505
  -2   145  -164
  -1   232   243

   L    FO    FC

H=    5,  K=   6

   0   291   317
   1   449   446
   2   414  -421
   3   -71  -121
   4   285   283
   5   -75  -100
   6   249  -260
   7   -72   -30
   8   166   105
   9   169   153
 -12   130   121
 -11   -73    63
 -10   226  -220
  -9   327  -317
  -8   -72   -26
  -7   490   494
  -6   205  -210
  -5   215  -205
  -4   156   171
  -3   -63   -80
  -2   595  -572
  -1   273  -303

H=    6,  K=   6

   0   345   373
   1   166  -149
   2   388  -397
   3   164   180
   4   113   -96
   5   350  -352
   6   -74    64
   7   165   191
   8   117    97
 -11   399  -393
 -10   319  -346
  -9   -71    -4
  -8   360   353
  -7   333  -306
  -6   -70   -63
  -5   147   129
  -4   527   540
  -3   530  -543
  -2    99   -83
  -1   797   793

H=    7,  K=   6

   0   152  -153
   1   -75   -36
   2   -77    34
   3   204   212
   4   -76     8
   5   109   -81
   6   128   113
   7   -78   -65
 -11   123  -135
 -10   326   347
  -9   -73    63
  -8   -73    14
  -7   -73    59
  -6   284   281
  -5   -72    39
  -4   254  -259
  -3   -71    16
  -2   312   280
  -1   105    88

H=    8,  K=   6

   0   -77   -44
   1   -78   -69
   2   150  -167
   3   138   174
   4   -75    82
   5   150  -176
   6   -79    60
 -10   -75    63

   L    FO    FC

  -9   -74    85
  -8   207   196
  -7   -72    44
  -6   396  -390
  -5   250   320
  -4   272   271
  -3   -75  -112
  -2   -75    52
  -1   231   241

H=    9,  K=   6

   0   312  -314
   1   214  -203
   2   175   144
   3   231   231
   4   184  -174
 -10   288   262
  -9   281   286
  -8   -76   -43
  -7   283  -263
  -6   319   318
  -5   -76    63
  -4   -77   -15
  -3   242  -220
  -2   140   143
  -1   -77   -51

H=   10,  K=   6

   0   -78   -73
   1   -79    89
   2   -79    51
   3   -82   -86
  -8   -77   -69
  -7   -77    11
  -6   -76   -71
  -5   159  -204
  -4   -76    14
  -3   131   102
  -2   -76     5
  -1   137  -117

H=   11,  K=   6

   0   183  -174
  -6   -80  -124
  -5   -81   103
  -4   -79   -72
  -3   163  -126
  -2   114    76
  -1   -80    13

H=    0,  K=   7

   1   469   470
   2   380   312
   3   -57    12
   4   297   289
   5   160  -171
   6   356   354
   7   121  -120
   8   -72    40
   9   176   184
  10   -71     9
  11   131   127

H=    1,  K=   7

   0   342  -312
   1   993   988
   2   374   327
   3   -59  -145
   4   430   404
   5   174   158
   6   175   196
   7   412  -408
   8   -74   -28
   9   543   523
  10   -73   -48

   L    FO    FC

  11   334  -363
 -11   269   262
 -10   -71    10
  -9   435  -403
  -8   102    57
  -7   201   224
  -6    93    39
  -5   314  -322
  -4   504   559
  -3   -56   100
  -2   225  -203
  -1   955  -949

H=    2,  K=   7

   0   818   847
   1    95    91
   2   438  -475
   3   -60   -13
   4    93   122
   5   302  -259
   6   580  -595
   7   -73   -11
   8   333   353
   9   -72   -24
  10   269  -275
 -11   196   195
 -10   447  -448
  -9   -72    63
  -8   528   494
  -7   -67    67
  -6   512  -500
  -5   427  -396
  -4   493   517
  -3   433  -411
  -2   532  -384
  -1   -56   -24

H=    3,  K=   7

   0   510  -512
   1   119    92
   2   194  -189
   3   204  -201
   4    94    85
   5   213  -224
   6   -71    43
   7   165  -159
   8   -73    53
   9   166   -54
  10   124  -111
 -12   -73    25
 -11   313  -316
 -10   208  -217
  -9   -71    76
  -8   -72  -121
  -7   116  -119
  -6   172   156
  -5   509   499
  -4   142   114
  -3   -59    54
  -2   128   -63
  -1   527   498

H=    4,  K=   7

   0   517   546
   1   170   172
   2   985 -1006
   3   328  -331
   4   441   471
   5   147  -173
   6   128  -146
   7   -74   -58
   8   120   166
   9   -75   -14
 -11   -72   109
 -10   342  -322
  -9   -72   -35
  -8   691   691
```

```
   L    FO    FC

  -7   154  -147
  -6   423  -432
  -5   100  -104
  -4   109   128
  -3   517  -498
  -2   297   260
  -1   335   345

 H=     5,  K=    7

   0   -66    -1
   1   816  -846
   2   -70    49
   3   361   387
   4   -73    15
   5   -75   -37
   6   -74   124
   7   292   275
   8   -75    20
 -11   281  -264
 -10   282  -297
  -9   697   696
  -8   -72   -17
  -7   624  -608
  -6   -65    32
  -5   562   360
  -4   248   236
  -3   245  -253
  -2   260   213
  -1   424   434

 H=     6,  K=    7

   0   226  -231
   1   277   272
   2   135  -131
   3   -75     5
   4   -77   127
   5   -74   -39
   6   -75    53
   7   -76    27
   8   -78    95
 -11   -74    41
 -10   282   294
  -9   159   164
  -8   107  -100
  -7   -73    18
  -6   297   307
  -5   -70   -48
  -4   414  -409
  -3   -59   -64
  -2   -69   -57
  -1   151   125

 H=     7,  K=    7

   0   174  -184
   1   200  -203
   2   -76   -58
   3   435   428
   4   140   153
   5   235  -239
   6   109    82
   7   187   171
 -11   179  -212
 -10   154  -154
  -9   298   275
  -8   -72   108
  -7   543  -537
  -6   203   201
  -5   425   405
  -4   -73    25
  -3   417  -411
  -2   272   280
  -1   -74    74

 H=     8,  K=    7

   0   -77  -122
   1   -77   -41

   L    FO    FC

   2   333   334
   3   -76   -20
   4   193  -190
   5   -76   -26
 -10   189   197
  -9   242   272
  -8   548  -567
  -7   -73   -77
  -6   588   579
  -5   -75    -3
  -4   385  -330
  -3   -75   -27
  -2   166   120
  -1   173  -153

 H=     9,  K=    7

   0   -77  -103
   1   -77    57
   2   -79   -70
   3   121   122
   4   -82    14
  -9   154  -168
  -8   -77   -95
  -7   -75   -70
  -6   -74     1
  -5   145  -159
  -4   -76     6
  -3   217   224
  -2   -75     5
  -1   -76     8

 H=    10,  K=    7

   0   -80  -103
   1   155    75
   2   151   168
  -8   365  -352
  -7   143  -155
  -6   417   413
  -5   115  -115
  -4   154  -137
  -3   -76    -9
  -2   206   178
  -1   145  -169

 H=    11,  K=    7

  -5   273  -248
  -4   -81   -34
  -3   224   179
  -2   -81    12

 H=     0,  K=    8

   0   918   895
   1   965   905
   2   112    64
   3   427  -445
   4   348   341
   5   256   289
   6   299  -277
   7   393  -331
   8   114    63
   9   199   188
  10   602  -633
  11   325  -345

 H=     1,  K=    8

   0   917   906
   1   462  -441
   2   -60   -75
   3   219   235
   4   -64   -19
   5   173  -185
   6   388  -332
   7   -73   -53
   8   -71   -49
   9   174  -178

   L    FO    FC

  10   -73    41
 -11   -74   -37
 -10   274  -280
  -9   293   301
  -8   131   100
  -7   115   -84
  -6   451  -429
  -5   -65     8
  -4   362   373
  -3   275  -279
  -2   713  -707
  -1   301   327

 H=     2,  K=    8

   0   356   349
   1   598   611
   2   247  -250
   3   310  -324
   4   154   181
   5   314   347
   6   125  -122
   7   439  -437
   8   157   131
   9   111    97
  10   193  -205
 -11   -73    64
 -10   -72   -74
  -9   -71    72
  -8   296   283
  -7   113  -108
  -6   -57   -44
  -5   663  -661
  -4   452   451
  -3   456   436
  -2   356  -395
  -1   291  -266

 H=     3,  K=    5

   0   497   500
   1   453  -458
   2   573  -562
   3   -66   -81
   4   294   296
   5   350  -361
   6   265  -250
   7   135   125
   8   229   231
   9   -74    40
 -11   198  -171
 -10   282  -314
  -9   720   721
  -8   292   281
  -7   159  -142
  -6   642  -637
  -5   588   607
  -4   560   539
  -3   424  -431
  -2   360  -381
  -1   187  -175

 H=     4,  K=    8

   0   -64   -58
   1   683  -698
   2   265   259
   3   143   166
   4   129  -154
   5   -73    64
   6   111   117
   7   -72    77
   8   -74    67
   9   115    99
 -11   146  -155
 -10   -70   -25
  -9   243   244
  -8   280  -273
  -7   107  -106
  -6   -69    20

   L    FO    FC

  -5   351   355
  -4   111    60
  -3   -65   -57
  -2   128   140
  -1   377   416

 H=     5,  K=    8

   0   347   364
   1   262  -261
   2   436  -457
   3   126   139
   4   143   117
   5   -74    30
   6   -74   -31
   7   -74    43
   8   219   200
 -11   -74   -75
 -10   131  -126
  -9   200   220
  -8   -72   121
  -7   358  -352
  -6   -71    18
  -5   -69   -49
  -4   407   412
  -3   334  -336
  -2   266  -237
  -1   291   313

 H=     6,  K=    8

   0   -72   -57
   1   359  -355
   2   172   137
   3   255   260
   4   -75   153
   5   -74    22
   6   145   164
   7   115    85
 -11   194  -153
 -10   259   240
  -9   222   241
  -8   597  -595
  -7   -75   -95
  -6   106   -44
  -5   385   375
  -4   351  -347
  -3   474  -458
  -2   358   376
  -1   363   353

 H=     7,  K=    8

   0   137  -202
   1   -75    44
   2   255   258
   3   -76  -105
   4   -75   -82
   5   -77    43
   6   -78    35
 -10   136   110
  -9   -73    63
  -8   -73   -97
  -7   158   135
  -6   -74    20
  -5   -75    77
  -4   282  -283
  -3   -74   -22
  -2   -75    58
  -1   123  -136

 H=     8,  K=    8

   0   -76   -56
   1   -76   -70
   2   123    63
   3   199   202
   4   -78   -69
   5   -81   -94
  -9   -76   -47
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```
   L     FO      FC
  -8    221    -227
  -7    -73     -32
  -6    317     304
  -5    137     129
  -4    -75      18
  -3    311    -318
  -2    144     151
  -1    -76      21

H=     9,  K=     8

   0    -78     -94
   1    -78      39
   2    227   . 206
   3    131    -127
  -8    213    -215
  -7    455     448
  -6    -76      58
  -5    -76     -18
  -4    185    -201
  -3    -76     105
  -2    203     191
  -1    152    -122

H=    10,  K=     8

   0    -80      53
   1    -80     133
  -7    -78      61
  -6    -79     -98
  -5    -78       9
  -4    -77     -24
  -3    146     131
  -2    -79       0
  -1    -81     -49

H=     0,  K=     9

   1    333    -308
   2    -62      32
   3    -63      27
   4    -66     -75
   5    -68     -38
   6    -71      96
   7    -72      42
   8    137    -160
   9    102      79
  10    -73     -23

H=     1,  K=     9

   0    604     597
   1    525     510
   2    119     -96
   3    222     231
   4    239     215
   5    -69     -25
   6    382    -395
   7    287    -297
   8    -72      -2
   9    184    -202
  10    163    -144
 -10    379    -369
  -9    188     192
  -8    -71    -119
  -7    199     192
  -6    -70     -70
  -5    101     -96
  -4    655     664
  -3    205     214
  -2    551    -550
  -1    555    -531

H=     2,  K=     9

   0    319     288
   1    286    -288
   2    363    -353
   3    400     409
   4    168     194

   L     FO      FC
   5    640    -669
   6    -72     -84
   7    276     270
   8    141     152
   9    104       4
 -11    232    -209
 -10    139     124
  -9    146     140
  -8    288    -316
  -7    113     110
  -6    440    -426
  -5    520     539
  -4    156     163
  -3    524    -513
  -2    237     236
  -1    -62      76

H=     3,  K=     9

   0    236     229
   1    -65       4
   2    135     151
   3    -68      23
   4    -71      -5
   5    -74     -58
   6    -73      93
   7    -73     -74
   8    -74     -46
   9    136     156
 -11    121    -128
 -10    -72     -71
  -9    105     116
  -8    226    -218
  -7    156    -172
  -6    -70      36
  -5    -69      46
  -4    128    -105
  -3    -65     -95
  -2     95     109
  -1    -64      71

H=     4,  K=     9

   0    269     305
   1    563    -592
   2    367    -387
   3    415     412
   4    -74      -5
   5    322    -331
   6    -72      -5
   7    240     230
   8    143     150
 -10    -73      97
  -9    496     489
  -8    213    -218
  -7    -73     -21
  -6    256    -246
  -5    116      94
  -4    203     222
  -3    345    -348
  -2    126    -131
  -1    212     194

H=     5,  K=     9

   0    198    -200
   1    220    -208
   2    380     383
   3    163     171
   4    294    -286
   5    -73     -65
   6    317     327
   7    -76      27
 -10    392     374
  -9    -72     -65
  -8    376    -388
  -7    313     335
  -6    -72     -72
  -5    268     277
  -4    344    -330

   L     FO      FC
  -3    145    -173
  -2    390     394
  -1    -71     -27

H=     6,  K=     9

   0    -74     -70
   1    175    -181
   2    -74     -30
   3    -74     -20
   4    -74      23
   5    -74     -37
   6    -76      33
 -10    -74      62
  -9    -73      52
  -8    154    -147
  -7    320     330
  -6    135     164
  -5    162    -152
  -4    -73     -72
  -3    -73      45
  -2    -73      78
  -1    -73      16

H=     7,  K=     9

   0    188    -173
   1    -76    -161
   2    245     240
   3    -76     122
   4    206    -193
   5    -78     -20
  -9    -75     -67
  -8    356    -359
  -7    235     243
  -6    -72       6
  -5    120     122
  -4    229    -199
  -3    257    -240
  -2    412     430
  -1    161     171

H=     8,  K=     9

   0    -74      15
   1    -76       8
   2    -77     117
   3    196    -187
   4    -77     -96
  -9    308    -291
  -8    -75      12
  -7    373     388
  -6    160    -167
  -5    120    -102
  -4    190    -181
  -3    277     281
  -2    -75      65
  -1    149    -163

H=     9,  K=     9

   0    -77     -43
   1    -79      56
   2    116     134
  -7    -79      96
  -6    153    -151
  -5    125     -73
  -4    -77     115
  -3    -76      39
  -2    -76     -36
  -1    -77     -30

H=    10,  K=     9

  -5    -79       6
  -4    -79     -26
  -3    -79      16
  -2    114      97
  -1    245    -233

   L     FO      FC
H=     0,  K=    10

   0    633     632
   1    573    -569
   2    357    -350
   3    418     412
   4    348     354
   5    -71      77
   6    347    -345
   7    -70     -24
   8    220     207
   9    295    -308
  10    273    -247

H=     1,  K=    10

   0    301    -303
   1    -65       4
   2    107     121
   3     99      67
   4    -70      42
   5    156    -165
   6    -72       5
   7    -72      76
   8    -71     -13
   9    -75    -111
 -10    218     225
  -9    131     121
  -8    -69     -33
  -7    125    -112
  -6    300    -301
  -5    390     389
  -4    193    -149
  -3    383    -377
  -2    165     154
  -1    282     280

H=     2,  K=    10

   0    -65      26
   1    231    -211
   2    113     -72
   3    -70      85
   4    296     284
   5    195    -193
   6    327    -301
   7    191    -187
   8    149     154
   9    -75      -4
 -10    235    -284
  -9    -71      36
  -8    -71     108
  -7    107     -91
  -6    -72     -97
  -5    167     204
  -4    457     437
  -3    145    -113
  -2    407    -398
  -1    -66      79

H=     3,  K=    10

   0    370    -363
   1    295    -313
   2    392     402
   3    229     167
   4    215    -242
   5    360    -375
   6    -71     -63
   7    271     284
   8    -74      57
 -10    -73      64
  -9    278     265
  -8    375    -374
  -7    377    -375
  -6    -71      30
  -5    548     542
  -4    -70     -37
  -3    357    -367
  -2    444     453
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```
   L     FO      FC

  -1    166     165

 H=     4,  K=   10

   0    108    -149
   1    134     143
   2    -72      37
   3    -74     -77
   4    107     -90
   5    -73     -18
   6    -73      -4
   7    -74      14
   8    -75      34
 -10    -75      46
  -9    159    -147
  -8    -71    -107
  -7    -71      21
  -6    -72     110
  -5    273     285
  -4    266    -264
  -3    138     110
  -2    -70      76
  -1    -70     -70

 H=     5,  K=   10

   0    146    -110
   1    193    -185
   2    164     154
   3    -74      77
   4    -73      20
   5    -73     -73
   6    -75      75
   7    129     124
 -10    154     143
  -9    420     433
  -8    134     -94
  -7    239    -226
  -6    -72      84
  -5    -73      22
  -4    172    -193
  -3    235    -217
  -2    146     158
  -1    356     365

 H=     6,  K=   10

   0    272    -264
   1    234     231
   2    147     168
   3    219    -220
   4    -73      42
   5    -75      60
   6    133     123
  -9    -75     -34
  -8    149    -148
  -7    296     290
  -6    196     163
  -5    -71      95
  -4    328    -314
  -3    -73      25
  -2    326     321
  -1    351    -358

 H=     7,  K=   10

   0    139     126
   1    -73      18
   2    -74     -83
   3    -76     -37
   4    -78      15
  -9    -75      -1
  -8    -74      43
  -7    -74      -6
  -6    -73      45
  -5    -73     -67
  -4    228    -251
  -3    240     243
  -2    129    -106
  -1    -74     -16
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```
   L     FO      FC

 H=     8,  K=   10

   0    130    -106
   1    -76      35
   2    -77      63
   3    -80    -120
  -8    243    -234
  -7    150     110
  -6    192     195
  -5    -76     -91
  -4    149    -130
  -3    137     107
  -2    -76     124
  -1    -75     -54

 H=     9,  K=   10

   0    135     154
   1    177     148
  -6    257    -239
  -5    122    -103
  -4    -77    -102
  -3    153     103
  -2    -77      23
  -1    141     -91

 H=     0,  K=   11

   1    -68     -81
   2    -68       7
   3    -70      75
   4    -72     -19
   5    -72      17
   6    173     179
   7    -70     -52
   8    102    -104
   9    168    -196

 H=     1,  K=   11

   0    313    -295
   1    455    -447
   2    -69     -15
   3    221     212
   4    125    -145
   5    -72      -8
   6    -71     -36
   7    -72      11
   8    216     236
   9    276    -292
  -9    240     235
  -8    -71     -10
  -7    279    -250
  -6    265    -286
  -5    -72      76
  -4    159     160
  -3    534    -524
  -2    118    -112
  -1    399     404

 H=     2,  K=   11

   0    392    -378
   1    369     362
   2    274     259
   3    -72      70
   4    454    -452
   5    159    -168
   6    192     175
   7    238     232
   8    321    -309
  -9    163    -175
  -8    269    -265
  -7    217    -215
  -6    -72      19
  -5    154     147
  -4    152    -127
  -3    -70     -21
  -2    360     378
```

```
   L     FO      FC

  -1    -69      43

 H=     3,  K=   11

   0    114     -52
   1    -71     -57
   2    172     201
   3    -73      49
   4    -73    -105
   5    -72      10
   6    -73      -3
   7    143    -157
   8    141     107
  -9    197    -165
  -8    161     186
  -7    -71    -104
  -6    -71       2
  -5    161     157
  -4    -72      45
  -3    -71     115
  -2    -71     -83
  -1    -71    -119

 H=     4,  K=   11

   0    200    -226
   1    277     295
   2    473     482
   3    123      83
   4    333    -329
   5    -73      42
   6    142      63
   7    -76       6
  -9    -73      24
  -8    352    -348
  -7    110     -71
  -6    313     304
  -5    409     447
  -4    109     -50
  -3    124    -125
  -2    294     294
  -1    -73     -39

 H=     5,  K=   11

   0    164    -170
   1    396     389
   2    132    -138
   3    234    -223
   4    -72     -35
   5    255     243
   6    -77      60
  -9    244    -224
  -8    162     165
  -7    363     380
  -6    -73     103
  -5    -71       4
  -4    -72     -76
  -3    -74      37
  -2    111     104
  -1    368    -401

 H=     6,  K=   11

   0    -72      77
   1    -72      58
   2    -73      45
   3    146    -115
   4    114     -62
   5    -77      45
  -8    208     200
  -7    145    -163
  -6    -71      14
  -5    -71     -15
  -4    160    -138
  -3    -72     -17
  -2    -73     -15
  -1    -73      56

 H=     7,  K=   11
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```
   L     FO      FC

   0    -74       0
   1    -76      94
   2    238    -266
   3    207    -203
  -8    -76      32
  -7    235     206
  -6    -74      32
  -5    280    -258
  -4    398    -437
  -3    216     199
  -2    147     131
  -1    290    -280

 H=     8,  K=   11

   0    190     195
   1    -75      84
   2    177    -161
  -6    418    -412
  -5    -78    -107
  -4    109      78
  -3    132      47
  -2    -76     -28
  -1    -76     -25

 H=     9,  K=   11

  -3    -78      55
  -2    -76      15

 H=     0,  K=   12

   0    -71     -90
   1    108      71
   2    117      66
   3    778     774
   4    501    -502
   5    199    -204
   6    144     132
   7    402     419
   8    152    -100

 H=     1,  K=   12

   0    -71      71
   1    -72      33
   2    -72     -26
   3    -71      43
   4    -72      42
   5    -71     -76
   6    267     253
   7    -72      27
   8    190    -219
  -8    234    -250
  -7    -71       6
  -6    184     193
  -5    255    -261
  -4    176    -175
  -3    243     227
  -2    581     593
  -1    -72      91

 H=     2,  K=   12

   0    -72      28
   1    154     178
   2    158    -158
   3    438     450
   4    205    -241
   5    241    -240
   6    232     246
   7    216     210
  -8    -73      -2
  -7    230    -242
  -6    100      73
  -5    351     356
  -4    -71     -30
  -3    187    -187
  -2    -72     -51
```

```
    L    FO     FC

   -1   160    140

 H=     3,  K=    12

    0   229    247
    1   -72     64
    2   -73   -126
    3   -72      6
    4   615   -617
    5   266    308
    6   224    252
    7   -77    -57
   -8   496   -492
   -7   -75    135
   -6   520    509
   -5   155   -171
   -4   514   -506
   -3   549    559
   -2   665    655
   -1   121    -91

 H=     4,  K=    12

    0   141   -125
    1   -72    -25
    2   -72      1
    3   -72    -36
    4   -74     20
    5   -75    -55
    6   -76     47
   -8   241    280
   -7   304    302
   -6   -70    -25
   -5   155   -151
   -4   263    265
   -3   -71    -46
   -2   173   -154
   -1   342   -319

 H=     5,  K=    12

    0   232   -240
    1   -72      2
    2   -72    -90
    3   150    178
    4   241   -243
    5   -77     36
   -8   122   -106
   -7   -74      6
   -6   270    259
   -5   -72    -75
   -4   186   -166
   -3   -72     90
   -2   -72     87
   -1   -72    -33

 H=     6,  K=    12

    0   142     66
    1   129   -123
    2   -75    -44
    3   -75    126
    4   -75    -19
   -7   331    325
   -6   103    -93
   -5   396   -401
   -4   -73    107
   -3   219    202
   -2   394   -405
   -1   507   -497

 H=     7,  K=    12

    0   144    155
    1   -76     47
    2   -77     39
   -6   228   -214
   -5   -75    -58
   -4   -75    106
   -3   143   -159
```

```
    L    FO     FC

   -2   -75     35
   -1   -78    141

 H=     8,  K=    12

   -4   -77     51
   -3   155    141
   -2   -77    -48
   -1   -77     27

 H=     0,  K=    13

    1   295    317
    2   200   -151
    3   110    -39
    4   -70      9
    5   -70     44
    6   119    -55
    7   112     82

 H=     1,  K=    13

    0   -72     71
    1   -71    -45
    2   -71     67
    3   177    184
    4   488   -483
    5   -70     42
    6   226    216
    7   136    115
   -7   177   -146
   -6   262    290
   -5   159   -180
   -4   338   -336
   -3   -72   -113
   -2   536    532
   -1   462    452

 H=     2,  K=    13

    0   -72    -23
    1   -70    -36
    2   261    237
    3   441   -436
    4   125    -69
    5   299    325
    6   -74    -63
   -7   202    237
   -6   137    177
   -5   293   -284
   -4   -72   -110
   -3   672    675
   -2   267    283
   -1   134   -128

 H=     3,  K=    13

    0   196   -205
    1   -72     23
    2   238   -236
    3   -73     67
    4   -72     14
    5   -75     39
    6   -75    -46
   -7   -75     44
   -6   -73    -51
   -5   -72    -28
   -4   -71     13
   -3   -70      5
   -2   -71      5
   -1   198   -175

 H=     4,  K=    13

    0   345   -329
    1   -72    -81
    2   -73     76
    3   145   -135
    4   201   -230
    5   365    393
```

```
    L    FO     FC

   -7   -74     39
   -6   257    250
   -5   255   -257
   -4   131    169
   -3   259    243
   -2   -72     39
   -1   373   -375

 H=     5,  K=    13

    0   129    155
    1   148    151
    2   -74     17
    3   209   -195
    4   211    279
   -7   107     48
   -6   212   -231
   -5   153   -113
   -4   217    226
   -3   -73     56
   -2   574   -572
   -1   353   -318

 H=     6,  K=    13

    0   110     80
    1   121     93
    2   -76     39
   -6   -75    -72
   -5   -74     35
   -4   -74     36
   -3   -74     38
   -2   -74    -30
   -1   -74    -40

 H=     7,  K=    13

    0   275    270
   -4   278    262
   -3   -76    -43
   -2   243   -254
   -1   -78   -120

 H=     0,  K=    14

    0   594   -615
    1   235   -239
    2   603    620
    3   -69     17
    4   365   -363
    5   114    119
    6   152    143

 H=     1,  K=    14

    0   -70    -77
    1   126     58
    2   -72    102
    3   258   -248
    4   -73    -96
    5   108     76
    6   -76    -17
   -6   131   -134
   -5   -73    -51
   -4   -72    -26
   -3   378    392
   -2   -72   -119
   -1   253   -230

 H=     2,  K=    14

    0   -72    -95
    1   125   -141
    2   238    224
    3   135   -129
    4   332   -353
    5   -75     35
   -6   -75    -59
   -5   -72    -51
   -4   229   -202
```

```
    L    FO     FC

   -3   -73    -79
   -2   445    441
   -1   154    155

 H=     3,  K=    14

    0   153   -179
    1   395    383
    2   135    171
    3   452   -431
    4   -76    -73
   -6   143   -154
   -5   295   -263
   -4   -73    102
   -3   316    308
   -2   -71    -25
   -1   539   -528

 H=     4,  K=    14

    0   147    150
    1   -74     75
    2   -75    -56
    3   -75    -64
   -6   175   -164
   -5   140    159
   -4   -74     27
   -3   -73     19
   -2   200   -196
   -1   -75     32

 H=     5,  K=    14

    0   -76    -73
    1   166    169
    2   -78    147
   -5   135    137
   -4   -74     52
   -3   -75     90
   -2   -73    -11
   -1   375   -391

 H=     6,  K=    14

   -3   -75    -64
   -2   224   -203
   -1   -76      1

 H=     0,  K=    15

    1   -72    -38
    2   -72     91
    3   118    119
    4   146    175

 H=     1,  K=    15

    0   121    -74
    1   276    258
    2   234    223
    3   188   -175
    4   112   -133
   -4   198   -189
   -3   233    221
   -2   178    196
   -1   165   -184

 H=     2,  K=    15

    0   273    258
    1   -72     -3
    2   155   -146
    3   152   -145
   -4   -74     40
   -3   236    244
   -2   212   -216
   -1   258   -208
   L    FO     FC       L    FO     FC       L    FO     FC       L    FO     FC

                       -3   -74     92       1   131     93       0   -72     -3
 H=    3,  K=  15      -2   -75    -81      -3   -77    130       1   272    231
                       -1   -76    102      -2   205   -130
   0  -73     58                            -1   -75    -99     H=    1,  K=  16
   1  -74     45     H=    4,  K=  15
   2  -75    -32                          H=    0,  K=  16        0   150    109
  -4  -75    112        0   125    150                            1   -75      7
```

```
   L     FO       FC

 H=     0,  K=     0

   2  1184  -1171
   4   -52     73
   6   616   -600
   8   205    229
  10   541   -559
  12   231    239

 H=     1,  K=     0

   1   887   -886
   3   243    274
   5   382    363
   7   -60    -64
   9   111    -87
  11   -79     19
 -11   537   -540
  -9   682    679
  -7   -57    -81
  -5   235    207
  -3   266   -289
  -1  1163   1194

 H=     2,  K=     0

   0  1193   1232
   2  1220  -1182
   4   -54      7
   6   275   -279
   8   349    359
  10   456   -472
 -12   176   -174
 -10   -68     -2
  -8   207    184
  -6   226   -190
  -4   266    262
  -2   645   -622

 H=     3,  K=     0

   1  5679  -5845
   3   716    718
   5   716   -698
   7   544    553
   9   -82   -100
  11   226    206
 -13   -86    164
 -11   243   -240
  -9   552    530
  -7   466   -462
  -5  1606   1557
  -3   259   -256
  -1   125    113

 H=     4,  K=     0

   0   342   -344
   2   217    210
   4   -61   -102
   6   123   -144
   8   -83     63
  10   -83    -29
 -12   448   -434
 -10   681    674
  -8   935   -923
  -6   200   -179
  -4   -53      7
  -2   -53    126

 H=     5,  K=     0

   1  1016  -1015
   3  1120   1093
   5   142    -96
   7   -75     69
   9   -85    -93
 -11   -83     66
  -9   234    240

   L     FC       FC

  -7   250   -273
  -5   -58     78
  -3   341   -342
  -1   241    248

 H=     6,  K=     0

   0   734   -709
   2  2412   2415
   4   -69    -37
   6   183    191
   8   252   -257
 -12   309   -306
 -10   498    507
  -8   484   -470
  -6   -63    -51
  -4   753   -786
  -2   567    540

 H=     7,  K=     0

   1   229    233
   3   -73      1
   5   -76    -74
   7   -85     34
 -11   321    307
  -9   405   -410
  -7   628    632
  -5   197    185
  -3   137    120
  -1   192   -198

 H=     8,  K=     0

   0   -72     69
   2   314    332
   4   495   -514
   6   170    174
 -10   -91   -136
  -8   250   -232
  -6   272    277
  -4   188   -178
  -2   350    357

 H=     9,  K=     0

   1   239    254
   3   973  -1001
   5   -92    151
 -11   -97     74
  -9   337   -342
  -7   592    602
  -5   326   -335
  -3   334    359
  -1   -76    -51

 H=    10,  K=     0

   0   -94     90
   2   172   -155
   4   -94     -2
 -10   252   -225
  -8   217    229
  -6   313   -335
  -4   -96    -38
  -2   -97   -139

 H=    11,  K=     0

   1   -97     60
  -7   187    183
  -5   -99    -92
  -3   -97      0
  -1   172   -204

 H=    12,  K=     0

  -6   262   -250
  -4   266    237
  -2   305   -291

   L     FO       FC

 H=     0,  K=     1

   1   111      3
   2   764   -816
   3   536   -548
   4   -52     20
   5    79    -18
   6   387   -407
   7   -59     62
   8   -63     47
   9   -67     56
  10   108    -94
  11   -76    -47
  12   -79     21

 H=     1,  K=     1

   0  1228   1246
   1   955   -966
   2   360   -342
   3   627   -588
   4   167    155
   5   659   -666
   6   887   -872
   7   -61    106
   8   520    514
   9   318   -300
  10   399   -391
  11   142    170
  12   245    253
 -12   190    154
 -11   253   -241
 -10   200   -178
  -9   214    219
  -8    97   -104
  -7   -57    -64
  -6   466   -451
  -5   277    296
  -4   537    561
  -3   599   -579
  -2   330    346
  -1  1110   1004

 H=     2,  K=     1

   0   989  -1015
   1   783   -764
   2   286    291
   3   674   -620
   4   -55    -67
   5   386   -385
   6   386    407
   7   553    554
   8   270   -268
   9   141   -113
  10   164    178
  11   -81    110
 -13   199    211
 -12   181   -178
 -11   259   -279
 -10   -68    106
  -9   343    336
  -8   319   -311
  -7   573   -552
  -6   -54     94
  -5  1369   1343
  -4  1140  -1092
  -3   979   -875
  -2   287   -303
  -1   893    836

 H=     3,  K=     1

   0   205   -190
   1   -56     11
   2   254    265
   3   201    197
   4   278    315
   5   -59    -47

   L     FO       FC

   6   146   -105
   7   284    301
   8   130     62
   9   -83    -47
  10   -81    -36
  11   -85     88
 -13   116     52
 -12   252   -272
 -11   -79    -42
 -10   -68     13
  -9   -65     -3
  -8   143   -110
  -7   172    169
  -6   -55     43
  -5   634   -626
  -4   -51    -37
  -3   -52     -5
  -2   373    370
  -1   732   -754

 H=     4,  K=     1

   0   984   -921
   1  1116  -1125
   2  1094   1061
   3   726    697
   4   116   -123
   5   344   -342
   6   461    479
   7   503    491
   8   -84    -50
   9   192   -209
  10   127    101
 -13   -85    -38
 -12   -84     92
 -11   -83    -96
 -10   307    283
  -9   319    301
  -7   195   -210
  -6   156    198
  -5   598    574
  -4    79     96
  -3   -53    -52
  -2    84    134
  -1   603   -559

 H=     5,  K=     1

   0   884   -862
   1  1014   1004
   2   980    966
   3   555   -567
   4   -64     20
   5   -70     79
   6   -73     93
   7   -74    -63
   8   -86   -161
   9   -84     46
  10   -88     63
 -12   289   -290
 -11   274    281
 -10   429    452
  -9   272   -269
  -8   529   -537
  -7   516    497
  -6   600    580
  -5   -57    -99
  -4   901   -878
  -3   586    563
  -2   478    496
  -1   219    219

 H=     6,  K=     1

   0   147    147
   1   -62    -71
   2   246    238
   3   -66    -42
   4   -69     19
   5   -73    -96
  L     FO      FC

  6    121     -37
  7    -85      58
  8    -86    -154
  9    -89    -103
-12    -89      -8
-11    322     320
-10    -87       9
 -9    -71     -19
 -8    102     -68
 -7    -65      62
 -6    136    -121
 -5    -60     -84
 -4    446     473
 -3    -58      88
 -2    -58      23
 -1    -59     -38

H=      7,  K=    1

  0    -65      27
  1    581     576
  2    523     529
  3    518    -520
  4    233    -258
  5    -88      51
  6    180     155
  7    255    -260
  8    292    -292
-12    -94     -81
-11    -91     -26
-10    -89      77
 -9    -94    -123
 -8    -74     -60
 -7    271     245
 -6    154     149
 -5    165    -177
 -4    744    -729
 -3    269     268
 -2    465     454
 -1    381    -388

H=      8,  K=    1

  0    125    -126
  1    213     238
  2    347    -364
  3    353    -373
  4    251     249
  5    -88      66
  6    159    -126
  7    -91    -102
-11    236     270
-10    267    -257
 -9    330    -335
 -8    178     190
 -7    406     408
 -6    365    -377
 -5    523    -539
 -4    260     268
 -3    677     671
 -2    448    -455
 -1    259    -267

H=      9,  K=    1

  0    123      40
  1    -77     -19
  2    -92      46
  3    208    -211
  4    -90     -94
  5    -93      46
  6    -93      91
-11    -98      -6
-10    257    -258
 -9    -92      43
 -8    -94      28
 -7    -94      40
 -6    -75      38
 -5    -75     -28
 -4    -76     -78

  L     FO      FC

 -3    142    -102
 -2    -76      13
 -1    -76     -36

H=     10,  K=    1

  0    196     242
  1    -93     101
  2    367    -367
  3    349    -352
  4    335     334
-10    -99    -114
 -9    226    -222
 -8    203     229
 -7    202     178
 -6    138    -173
 -5    -95    -116
 -4    -96     -23
 -3    300     304
 -2    -97    -109
 -1    221    -205

H=     11,  K=    1

  0   -100     162
  1    -99     -33
  2    163    -129
 -8    265     280
 -7    150    -146
 -6    211    -200
 -5    -99     111
 -4    171     169
 -3    -98     -44
 -2    243    -251
 -1    171     231

H=     12,  K=    1

 -6   -102      15
 -5   -103       2
 -4   -103       0
 -3   -102      75
 -2   -102     -26
 -1   -104     -94

H=      0,  K=    2

  0    885    -907
  1   1157   -1127
  2    200    -185
  3   1413    1389
  4    121     107
  5    581    -628
  6    695    -686
  7    448     423
  8    329     319
  9    463    -466
 10    -77      32
 11    298     306
 12    125      89

H=      1,  K=    2

  0    824    -819
  1    313     321
  2    671     724
  3    720    -706
  4    107     -87
  5    -54     -62
  6    266     261
  7    -62     -42
  8    -66      51
  9    -71     -98
 10    -78     -32
 11    -78      -6
 12    -82      22
-12    398    -396
-11    -76      78
-10    126     112
 -9    153    -118

  L     FO      FC

 -8    123    -181
 -7    354    -341
 -6    999     983
 -5    538     537
 -4    349    -341
 -3    -53     -40
 -2    440    -460
 -1    137     198

H=      2,  K=    2

  0    288    -306
  1    890    -892
  2    -55     -78
  3    346    -310
  4     84      92
  5    422    -376
  6    364    -400
  7    871     861
  8    258     264
  9    319    -329
 10    -80      60
 11    -81     109
-12    -79     -97
-11    -76       3
-10    -68     -11
 -9    100    -149
 -8    101     114
 -7    -57     -78
 -6     99     114
 -5    807     825
 -4    -51      45
 -3    369    -326
 -2    693     676
 -1   1040    1011

H=      3,  K=    2

  0    558     472
  1    661     648
  2    546     511
  3    -55      91
  4   1147   -1163
  5    -60     -50
  6    735     758
  7    339     362
  8    276    -304
  9    134    -122
 10    154     133
 11    -86     -50
-13    -83     -14
-12    466    -465
-11    -81     -91
-10    262     248
 -9    -66     -17
 -8    595    -605
 -7    546    -552
 -6   1062    1011
 -5    922     896
 -4   1531   -1495
 -3    108     -93
 -2   1009     951
 -1    119     103

H=      4,  K=    2

  0    -54     -38
  1    113     126
  2     99     -57
  3    277    -275
  4    278     273
  5    207     205
  6    112      50
  7    114    -118
  8    -83      42
  9    127     -91
 10    -85      38
-12    119     -94
-11    425     460
-10    108     -75

  L     FO      FC

 -9    163    -155
 -8    163     140
 -7    223     227
 -6    370     361
 -5    689    -687
 -4    377    -344
 -3    117    -109
 -2    262    -280
 -1    617     616

H=      5,  K=    2

  0    717    -673
  1    -59      52
  2    765     779
  3    -62      62
  4    -66    -137
  5    -70     -15
  6    205     213
  7    -75     133
  8    270    -311
  9    130    -134
 10    153     167
-12    239    -238
-11    -86      94
-10    154     237
 -9    -70      49
 -8    -67      31
 -7    143    -135
 -6     92      85
 -5    127    -147
 -4    541    -563
 -3    115     136
 -2    109      98
 -1    411    -391

H=      6,  K=    2

  0    -62     -98
  1    141     117
  2    208    -213
  3    164    -193
  4    -71     -28
  5    244     245
  6    -76     -40
  7    302    -317
  8    -86    -126
  9    180     211
-12    -90     -20
-11    673     684
-10    147     102
 -9    393    -403
 -8    -69      38
 -7    230     301
 -6    412     409
 -5    298    -279
 -4    601    -584
 -3   1095    1070
 -2    -60      55
 -1   1045   -1030

H=      7,  K=    2

  0    171    -177
  1    -69     -31
  2    -70       5
  3    -74       9
  4    -76       9
  5    -91     -81
  6    -87     -78
  7    -90     -43
  8    -92      63
-12    189     194
-11    -92      95
-10    292    -297
 -9    -91      19
 -8    -73     -22
 -7    153    -154
 -6    198    -203
 -5    209    -207
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L	FO	FC
-4	369	371
-3	147	142
-2	-64	16
-1	174	193
H=	8, K=	2
0	168	177
1	171	130
2	-76	-64
3	195	-199
4	-88	0
5	126	130
6	-90	1
7	207	-238
-11	218	211
-10	-94	-78
-9	166	-202
-8	-93	35
-7	116	51
-6	-73	52
-5	202	-193
-4	-71	12
-3	403	412
-2	-72	-55
-1	-72	-80
H=	9, K=	2
0	254	257
1	-79	27
2	-94	-118
3	-91	63
4	257	253
5	-93	30
6	175	-178
-11	-97	25
-10	362	-396
-9	-93	-84
-8	373	387
-7	-95	-29
-6	509	-513
-5	180	-191
-4	318	315
-3	275	255
-2	401	-401
-1	-77	-5
H=	10, K=	2
0	-93	-61
1	-93	42
2	-94	-6
3	-95	11
4	-98	11
-10	-100	-87
-9	143	189
-8	141	57
-7	-96	30
-6	-95	81
-5	176	202
-4	-97	66
-3	201	-201
-2	-95	-6
-1	-95	31
H=	11, K=	2
0	145	150
1	-99	-40
2	-100	-159
-8	262	189
-7	-102	-51
-6	-100	-48
-5	-99	18
-4	-98	34
-3	-99	8
-2	155	-155
-1	-97	2

L	FO	FC
H=	12, K=	2
-6	-102	34
-5	259	234
-4	-104	61
-3	284	-272
-2	-102	-104
-1	333	328
H=	0, K=	3
1	415	441
2	441	386
3	656	633
4	486	-500
5	-54	-51
6	-56	-1
7	253	-241
8	-64	18
9	133	-121
10	-76	16
11	-75	46
12	-78	6
H=	1, K=	3
0	189	180
1	272	-197
2	-55	-60
3	311	-260
4	369	-390
5	99	-45
6	374	346
7	682	689
8	338	-319
9	382	-383
10	561	559
11	-79	-2
12	116	-82
-12	184	-206
-11	143	110
-10	243	256
-9	-67	10
-8	215	-216
-7	-58	-70
-6	341	346
-5	-53	10
-4	408	-384
-3	705	-709
-2	198	-238
-1	283	230
H=	2, K=	3
0	334	-309
1	151	-133
2	270	-277
3	493	501
4	247	-221
5	255	240
6	231	241
7	414	-404
8	310	-331
9	233	246
10	-79	74
11	-82	-117
-12	216	-205
-11	-76	4
-10	187	-194
-9	603	-617
-8	216	-230
-7	292	290
-6	955	915
-5	425	-416
-4	487	-455
-3	872	897
-2	425	427
-1	460	-444
H=	3, K=	3

L	FO	FC
0	232	-260
1	296	303
2	486	-514
3	347	-366
4	392	-386
5	171	192
6	194	195
7	158	143
8	-72	62
9	-82	-59
10	-83	79
11	-85	-13
-12	133	30
-11	-78	20
-10	-81	34
-9	-67	2
-8	157	159
-7	-60	49
-6	138	142
-5	90	12
-4	-52	53
-3	432	-418
-2	393	-373
-1	140	154
H=	4, K=	3
0	-54	-28
1	183	211
2	424	416
3	228	-246
4	267	-272
5	310	307
6	302	293
7	217	-221
8	351	-360
9	151	157
10	172	163
-12	183	-217
-11	125	188
-10	199	-219
-9	457	-455
-8	233	-234
-7	557	537
-6	354	350
-5	382	-397
-4	108	45
-3	-53	3
-2	152	196
-1	260	213
H=	5, K=	3
0	488	474
1	657	681
2	457	-455
3	224	-231
4	-66	24
5	125	115
6	-75	-82
7	-87	-42
8	-84	107
9	-87	138
-12	-87	88
-11	332	340
-10	137	-25
-9	-71	48
-8	668	677
-7	325	329
-6	313	-323
-5	753	-740
-4	133	162
-3	205	213
-2	421	-462
-1	495	-492
H=	6, K=	3
0	118	-167

L	FO	FC
1	294	300
2	-66	-54
3	186	198
4	151	141
5	-76	97
6	-88	-45
7	-87	-114
8	-90	-124
9	-91	38
-12	-91	106
-11	-88	-92
-10	-87	-53
-9	-72	-24
-8	-71	-5
-7	-68	-97
-6	-65	-7
-5	-63	-72
-4	-61	11
-3	93	-92
-2	210	172
-1	-61	42
H=	7, K=	3
0	-68	63
1	-70	71
2	142	-155
3	-74	-75
4	-77	99
5	-90	80
6	163	-140
7	259	-245
8	169	149
-12	184	186
-11	253	269
-10	144	-141
-9	296	323
-8	242	252
-7	-72	51
-6	446	-447
-5	420	-425
-4	565	572
-3	466	486
-2	335	-313
-1	465	-461
H=	8, K=	3
0	125	152
1	156	-116
2	162	-148
3	226	192
4	-90	111
5	-90	-90
6	-94	-133
7	-94	97
-11	-96	-111
-10	250	-238
-9	-90	-1
-8	-93	-105
-7	430	-430
-6	356	-353
-5	254	269
-4	717	720
-3	215	-231
-2	313	-309
-1	249	276
H=	9, K=	3
0	132	-19
1	-95	59
2	154	-148
3	-93	-43
4	-94	-3
5	-95	28
-10	179	85
-9	-95	43
-8	-94	-32
-7	-94	41

L	FO	FC
-6	-96	30
-5	147	-124
-4	133	143
-3	-78	67
-2	-78	-8
-1	-78	-23
H=	10, K=	3
0	197	225
1	-94	-119
2	-96	-154
3	166	165
4	144	135
-9	199	226
-8	-95	-33
-7	212	-239
-6	161	-139
-5	235	245
-4	207	230
-3	247	-263
-2	183	-218
-1	184	193
H=	11, K=	3
0	184	-160
1	-102	-118
2	158	76
-8	-101	-75
-7	-102	67
-6	268	234
-5	-101	133
-4	-98	-59
-3	280	-287
-2	-98	62
-1	202	195
H=	12, K=	3
-5	-102	-40
-4	-103	58
-3	-104	-95
-2	-104	-87
H=	0, K=	4
0	2251	-2102
1	262	-270
2	739	765
3	424	404
4	273	-313
5	-55	74
6	529	545
7	311	285
8	688	-698
9	214	200
10	250	273
11	266	-261
12	133	-138
H=	1, K=	4
0	537	565
1	538	505
2	852	-806
3	115	-159
4	320	345
5	-56	50
6	-59	-20
7	104	-110
8	-67	-56
9	210	198
10	-78	-42
11	-80	49
-12	-79	-72
-11	-78	10
-10	248	-243
-9	524	-514
-8	95	70

L	FO	FC
-7	-60	90
-6	119	130
-5	767	-752
-4	-52	6
-3	1065	1044
-2	146	-117
-1	289	-287
H=	2, K=	4
0	764	-745
1	600	590
2	405	406
3	269	-265
4	745	-730
5	-59	-3
6	560	583
7	134	110
8	277	-272
9	129	20
10	396	391
11	139	-156
-12	-80	34
-11	173	-173
-10	-78	-68
-9	-69	-99
-8	336	-315
-7	115	-115
-6	400	374
-5	111	86
-4	449	-454
-3	77	106
-2	458	454
-1	609	-543
H=	3, K=	4
0	81	-55
1	737	725
2	126	132
3	630	-650
4	166	-175
5	726	738
6	-66	-27
7	467	-491
8	217	-191
9	307	329
10	162	-163
11	-85	-46
-12	-81	-11
-11	-80	93
-10	416	-427
-9	265	-241
-8	240	210
-7	1136	1105
-6	410	419
-5	1222	-1187
-4	-54	35
-3	376	369
-2	262	250
-1	192	161
H=	4, K=	4
0	161	-170
1	263	-293
2	136	-122
3	246	278
4	141	134
5	-67	-136
6	-71	-78
7	108	97
8	-84	25
9	-83	-46
10	-86	-33
-12	195	229
-11	-82	60
-10	-82	-51
-9	310	324
-8	721	720

L	FO	FC
-7	-62	-16
-6	-60	-22
-5	148	-139
-4	496	480
-3	278	-232
-2	473	-487
-1	302	282
H=	5, K=	4
0	-59	96
1	703	710
2	149	-147
3	550	-558
4	138	147
5	437	442
6	-75	-75
7	178	-183
8	-85	4
9	-88	82
-12	-89	-94
-11	146	116
-10	-87	199
-9	110	-128
-8	-69	97
-7	367	350
-6	187	184
-5	285	-262
-4	-59	45
-3	282	299
-2	107	-99
-1	345	-325
H=	6, K=	4
0	428	410
1	122	86
2	428	-424
3	102	-85
4	146	147
5	-75	-20
6	278	-256
7	-87	89
8	200	227
-12	460	452
-11	-88	56
-10	272	-296
-9	439	456
-8	207	219
-7	283	-301
-6	549	-552
-5	230	-219
-4	484	493
-3	-62	-53
-2	527	-508
-1	-62	-87
H=	7, K=	4
0	139	-165
1	-71	41
2	159	156
3	-75	13
4	-76	-54
5	-90	-1
6	-89	-5
7	-91	30
8	-92	-31
-11	144	-120
-10	-91	-44
-9	-91	-26
-8	337	-342
-7	549	-542
-6	-71	59
-5	-69	2
-4	-69	64
-3	248	-268
-2	101	110
-1	275	259

L	FO	FC
H=	8, K=	4
0	122	106
1	-77	-60
2	199	-188
3	-93	70
4	201	227
5	-90	-44
6	298	-303
-11	-96	88
-10	-93	-81
-9	-90	-44
-8	-93	88
-7	241	-240
-6	274	-277
-5	-75	-149
-4	269	304
-3	-73	44
-2	287	-230
-1	-74	20
H=	9, K=	4
0	-95	-24
1	-98	-175
2	-94	-35
3	280	298
4	-94	69
5	221	-187
-10	156	-56
-9	185	192
-8	295	-318
-7	350	-361
-6	234	220
-5	552	560
-4	-79	99
-3	187	-186
-2	-78	49
-1	169	117
H=	10, K=	4
0	-96	-106
1	-95	26
2	-95	23
3	-95	-34
4	-95	-29
-9	-97	52
-8	-97	-16
-7	178	173
-6	327	339
-5	-94	-38
-4	-94	-34
-3	-93	43
-2	139	115
-1	-94	-48
H=	11, K=	4
0	-100	43
1	-104	-166
-7	-102	-42
-6	241	245
-5	161	90
-4	-99	-7
-3	-100	-113
-2	-101	-12
-1	180	177
H=	12, K=	4
-3	-104	-46
H=	0, K=	5
1	123	146
2	383	388
3	-52	67
4	302	-309
5	126	-128

L	FO	FC
6	93	104
7	111	-87
8	255	-255
9	254	-227
10	202	196
11	110	-50
12	118	-42
H= 1, K= 5		
0	713	-737
1	201	219
2	242	-235
3	591	-565
4	283	-284
5	725	732
6	-60	14
7	300	-318
8	244	-239
9	276	261
10	-77	24
11	137	-129
-12	171	-146
-11	-77	61
-10	-76	-44
-9	334	-321
-8	-65	73
-7	-63	90
-6	181	179
-5	585	-566
-4	545	-525
-3	1716	1673
-2	1175	1122
-1	242	-233
H= 2, K= 5		
0	491	542
1	227	249
2	89	58
3	508	-492
4	874	855
5	391	390
6	321	-351
7	358	-375
8	189	195
9	122	129
10	223	-214
11	-82	-1
-12	175	194
-11	119	77
-10	-77	-74
-9	154	198
-8	242	251
-7	178	152
-6	311	-304
-5	195	-206
-4	920	899
-3	929	865
-2	1147	-1055
-1	-52	52
H= 3, K= 5		
0	147	166
1	336	-337
2	291	-300
3	129	-169
4	110	-84
5	369	379
6	163	139
7	174	-171
8	-83	-9
9	161	167
10	141	127
-12	145	146
-11	-80	-34
-10	-80	42
-9	175	188
-8	354	338

L	FO	FC
-7	273	-275
-6	-59	87
-5	161	168
-4	227	226
-3	88	-92
-2	120	-137
-1	292	282
H= 4, K= 5		
0	379	392
1	621	630
2	349	-323
3	334	-358
4	401	412
5	539	546
6	488	-502
7	127	-113
8	160	191
9	-83	74
10	159	-142
-12	-84	34
-11	122	99
-10	-81	-32
-9	-70	60
-8	547	551
-7	188	155
-6	241	-227
-5	338	-323
-4	492	486
-3	177	185
-2	1320	-1288
-1	510	-501
H= 5, K= 5		
0	333	333
1	555	-589
2	514	-523
3	254	239
4	365	362
5	370	-382
6	-75	-81
7	-86	60
8	131	113
9	-89	-67
-12	386	402
-11	253	-241
-10	239	-254
-9	-86	49
-8	-69	7
-7	293	-310
-6	188	-175
-5	290	286
-4	-59	23
-3	555	-576
-2	659	-626
-1	736	703
H= 6, K= 5		
0	-64	-4
1	-66	-12
2	160	129
3	-72	73
4	-75	56
5	-76	82
6	194	-187
7	-87	-86
8	-91	119
-12	251	-223
-11	169	-162
-10	-87	114
-9	-87	-43
-8	149	-120
-7	277	-299
-6	-69	74
-5	102	-50
-4	113	-141
-3	221	-211

L	FC	FC
-2	-63	-5
-1	-64	14
H= 7, K= 5		
0	449	455
1	246	-263
2	259	-265
3	160	170
4	-91	102
5	207	-198
6	287	-300
7	262	273
-11	-92	-48
-10	-91	-112
-9	-89	-96
-8	231	-236
-7	377	-387
-6	-73	-101
-5	326	321
-4	493	472
-3	553	-566
-2	476	-479
-1	807	803
H= 8, K= 5		
0	333	-332
1	115	-47
2	215	200
3	203	188
4	139	-133
5	154	-197
6	189	178
-11	323	-320
-10	155	213
-9	-91	124
-8	-92	35
-7	-92	-69
-6	217	206
-5	372	368
-4	280	-276
-3	271	-269
-2	450	472
-1	347	348
H= 9, K= 5		
0	-95	-20
1	-94	-19
2	-93	-38
3	-94	7
4	-96	65
5	-97	-81
-10	161	137
-9	-96	-140
-8	-93	63
-7	-95	82
-6	-95	101
-5	-95	73
-4	-96	127
-3	-96	3
-2	-97	101
-1	-96	14
H= 10, K= 5		
0	372	-385
1	286	-273
2	159	178
3	257	242
-9	265	236
-8	-98	-11
-7	-96	13
-6	246	243
-5	150	141
-4	-96	-153
-3	160	-164
-2	238	284
-1	144	168

L	FO	FC
H= 11, K= 5		
0	215	-220
1	174	173
-7	-104	14
-6	-102	-2
-5	-102	-92
-4	170	-139
-3	-101	66
-2	162	149
-1	240	-240
H= 0, K= 6		
0	1014	-956
1	1111	1118
2	230	-256
3	1401	-1373
4	349	344
5	494	479
6	-62	103
7	379	-403
8	-68	56
9	376	407
10	287	276
11	148	-165
H= 1, K= 6		
0	658	625
1	257	239
2	76	-93
3	-55	44
4	342	321
5	439	-420
6	-62	-36
7	-67	-59
8	-70	55
9	-80	127
10	-78	-13
11	-82	38
-11	-78	32
-10	-76	-122
-9	-77	-56
-8	410	414
-7	106	103
-6	669	-660
-5	194	188
-4	954	952
-3	107	117
-2	900	-823
-1	-52	-105
H= 2, K= 6		
0	200	-163
1	675	662
2	124	-125
3	667	-631
4	108	104
5	713	706
6	-65	-3
7	518	-521
8	203	-192
9	376	377
10	-81	61
11	-83	-93
-12	-79	-16
-11	-77	39
-10	-76	-12
-9	-69	11
-8	177	-175
-7	189	230
-6	-61	48
-5	332	-323
-4	284	235
-3	772	736
-2	266	256
-1	358	-381

```
   L    FO     FC

H=    3,  K=    6

   0   190    189
   1   543    541
   2   631   -646
   3   366    386
   4  1168   1161
   5   168   -204
   6   569   -567
   7   114    -60
   8   275    287
   9   -82    -42
  10   145   -137
 -12   257    263
 -11   138    122
 -10   146   -103
  -9   326   -304
  -8   554    557
  -7   -65     42
  -6   756   -747
  -5   316   -317
  -4   913    886
  -3   356   -356
  -2  1062  -1011
  -1   142    134

H=    4,  K=    6

   0   -57    -37
   1   179   -198
   2   324   -320
   3   -63     39
   4   -67     19
   5   228   -222
   6   314    291
   7   -86      4
   8   -83    -22
   9   -86     53
 -12   -86     42
 -11   495   -488
 -10   -81     20
  -9   139    174
  -8   -70     29
  -7   534   -549
  -6    97    -21
  -5   566    608
  -4   334   -317
  -3   590   -581
  -2    85     90
  -1   356    371

H=    5,  K=    6

   0   446    468
   1   210    218
   2   621   -632
   3   -68      2
   4   490    500
   5   207   -194
   6   324   -325
   7   -85     50
   8   157    145
   9   -90     82
 -11   -88    -14
 -10   196   -191
  -9   -86   -106
  -8   110     75
  -7   307    330
  -6   230   -254
  -5   -65     -8
  -4   187    203
  -3   327   -311
  -2   582   -605
  -1   -60    -71

H=    6,  K=    6

   0   -68     85
   1   341   -351
```

```
   L    FO     FC

   2   272   -274
   3   305    318
   4   244   -253
   5   386   -408
   6   204    195
   7   228    232
   8   -90    -25
 -11   439   -440
 -10   136   -130
  -9   151    204
  -8   155    149
  -7   333   -346
  -6   -70     65
  -5   217    211
  -4   207    198
  -3   603   -615
  -2   200    226
  -1   912    910

H=    7,  K=    6

   0   224   -227
   1   -74    101
   2   -76     82
   3   114    102
   4   -92     11
   5   -90    -22
   6   -91     67
   7   -95    -74
 -11   -93    -60
 -10   362    383
  -9   -91    -56
  -8   -91    -63
  -7   -93    115
  -6   397    423
  -5   -72    -84
  -4   365   -372
  -3   114    105
  -2   342    337
  -1   -71    -14

H=    8,  K=    6

   0   132   -120
   1   201   -165
   2   -94    -33
   3   215    215
   4   -92     -7
   5   268   -282
   6   -98    106
 -10   -95     82
  -9   136    114
  -8   -91     26
  -7   -93    -50
  -6   237   -237
  -5   269    267
  -4   117    114
  -3   245   -237
  -2   142    139
  -1   387    401

H=    9,  K=    6

   0   323   -331
   1   -93    -14
   2   239    221
   3   -96    110
   4   277   -263
  -9   -97    102
  -8   212   -223
  -7   -95    -89
  -6   438    428
  -5   -93    -32
  -4   143   -178
  -3   -95    -73
  -2   244    234
  -1   158   -169

H=   10,  K=    6
```

```
   L    FO     FC

   0   -99    -32
   1  -100     97
   2  -100     -6
   3  -101    -61
  -8  -102    -25
  -7  -100     55
  -6   -99    -81
  -5   291   -274
  -4   -98    100
  -3   167    159
  -2   -99    -51
  -1   149   -148

H=   11,  K=    6

   0   298   -280
  -6  -104      1
  -5  -103     46
  -4  -102    -87
  -3  -102    -11
  -2  -102    104
  -1  -102    -54

H=    0,  K=    7

   1   423    425
   2   333    314
   3   -54    -14
   4   272    270
   5   -60      8
   6   285    292
   7   167   -188
   8   -69     25
   9   219    223
  10   130    123
  11   -79    -13

H=    1,  K=    7

   0   168    141
   1   879    858
   2   -55    -27
   3   -56    -22
   4   673    667
   5   -61    -27
   6   -65    -94
   7   279   -279
   8   298    278
   9   536    508
  10   274   -245
  11   293   -299
 -11   154    141
 -10   154   -141
  -9   244   -258
  -8   176    144
  -7   115    106
  -6   240   -249
  -5   192   -214
  -4   806    822
  -3   -55     -5
  -2   678   -665
  -1   651   -645

H=    2,  K=    7

   0   750    693
   1   237   -240
   2   236   -244
   3   231    225
   4   -60     -3
   5   456   -450
   6   428   -439
   7   243    234
   8   234    247
   9   151   -126
  10   200   -190
 -11   -79    -42
 -10   271   -277
  -9   254    275
  -8   505    488
```

```
   L    FO     FC

  -7   284   -267
  -6   414   -393
  -5   -59     29
  -4   362    342
  -3   847   -840
  -2   249   -272
  -1   336    341

H=    3,  K=    7

   0   446   -438
   1   138    138
   2   142   -153
   3   167   -203
   4   -65    108
   5   131   -141
   6   174   -170
   7   176   -185
   8   -83    152
   9   -84    -14
  10   146   -138
 -11   279   -289
 -10   -80    -49
  -9   139    172
  -8   196   -196
  -7   135   -105
  -6   207    210
  -5   432    444
  -4   -60     78
  -3   164    154
  -2   117   -118
  -1   364    361

H=    4,  K=    7

   0   251    282
   1   192   -200
   2   804   -827
   3   -65     88
   4   407    420
   5   442   -444
   6   131   -160
   7   154    111
   8   -85    130
   9   178   -181
 -11   -84    -43
 -10   161   -199
  -9   198    202
  -8   533    519
  -7   343   -323
  -6   290   -313
  -5   233    243
  -4    93     64
  -3   661   -683
  -2   348    334
  -1   606    628

H=    5,  K=    7

   0   289   -293
   1   766   -776
   2   304    330
   3   320    341
   4   152   -155
   5   -74    -35
   6   134    181
   7   230    199
   8   -92    -82
 -11   219   -218
 -10   -86     14
  -9   506    510
  -8   240   -253
  -7   567   -581
  -6   296    287
  -5   253    243
  -4   -64    -63
  -3   -65   -125
  -2   531    520
  -1   281    303
```

L	FO	FC
H= 6. K= 7		
0	122	-104
1	170	147
2	200	-214
3	-75	47
4	-91	130
5	-87	-46
6	-87	39
7	146	120
-11	-91	108
-10	294	288
-9	-86	48
-8	-90	-162
-7	-73	66
-6	207	217
-5	-71	-78
-4	354	-399
-3	-69	-45
-2	-69	-83
-1	177	144
H= 7. K= 7		
0	351	-367
1	188	-190
2	-79	115
3	338	324
4	-90	-77
5	137	-140
6	248	237
-10	-93	-7
-9	189	178
-8	-69	-78
-7	372	-401
-6	339	337
-5	260	279
-4	307	-315
-3	313	-315
-2	525	539
-1	-74	118
H= 8. K= 7		
0	-94	-66
1	-95	100
2	296	290
3	-93	-125
4	219	-144
5	-98	81
-10	-98	120
-9	-96	20
-8	415	-407
-7	151	118
-6	534	545
-5	188	-217
-4	329	-364
-3	192	199
-2	157	127
-1	361	-331
H= 9. K= 7		
0	-94	-74
1	-93	29
2	-95	-11
3	163	146
4	-99	-55
-9	164	-206
-8	-97	-23
-7	-95	35
-6	-94	-1
-5	-93	-77
-4	-95	-35
-3	214	176
-2	-95	16
-1	-95	14
H= 10. K= 7		
0	-101	-69
1	228	188
2	167	180
-7	-102	59
-6	399	398
-5	176	-205
-4	193	-136
-3	187	161
-2	-101	98
-1	282	-306
H= 11. K= 7		
-4	-105	90
-3	-104	157
-2	-102	-104
H= 0. K= 8		
0	1038	1036
1	437	404
2	172	-205
3	-57	-53
4	477	491
5	-63	-66
6	317	-306
7	-69	-82
8	173	176
9	-75	-13
10	579	-600
11	-79	-108
H= 1. K= 8		
0	614	607
1	530	-524
2	196	152
3	194	224
4	161	-163
5	192	-195
6	178	-181
7	112	-22
8	123	-149
9	-79	-70
10	-80	39
-11	181	-147
-10	149	-136
-9	405	407
-8	-79	-109
-7	256	-246
-6	227	-222
-5	301	295
-4	-60	100
-3	459	-438
-2	284	-272
-1	439	445
H= 2, K= 8		
0	510	499
1	362	325
2	348	-361
3	-60	31
4	263	273
5	-67	113
6	326	-339
7	259	-256
8	307	322
9	-82	-27
10	337	-336
-11	-83	-3
-10	-80	12
-9	-80	87
-8	178	144
-7	184	-202
-6	97	-78
-5	414	-433
-4	498	492
-3	171	148
-2	417	-425
-1	-57	-92
H= 3. K= 8		
0	169	156
1	493	-485
2	174	-183
3	125	131
4	137	-94
5	539	-537
6	-71	9
7	256	270
8	-82	86
9	128	-90
-11	209	-186
-10	-80	-54
-9	680	712
-8	-81	7
-7	321	-327
-6	235	-202
-5	675	675
-4	-62	82
-3	599	-603
-2	-60	-59
-1	100	-46
H= 4. K= 8		
0	138	-154
1	471	-487
2	296	316
3	-68	-16
4	173	-156
5	138	112
6	-86	134
7	-83	-20
8	-86	41
9	-90	127
-11	154	-103
-10	-84	147
-9	-83	106
-8	471	-477
-7	-70	106
-6	197	193
-5	188	165
-4	144	-141
-3	151	141
-2	206	207
-1	113	128
H= 5. K= 8		
0	104	153
1	419	-440
2	239	-256
3	343	368
4	-74	-43
5	156	-136
6	-86	21
7	160	145
8	-92	88
-11	-90	-63
-10	-88	-10
-9	-88	143
-8	-87	19
-7	252	-243
-6	-70	66
-5	-69	28
-4	284	307
-3	372	-383
-2	-66	0
-1	322	330
H= 6. K= 8		
0	261	-266
1	138	-134
2	336	337
3	108	104
4	-89	9
5	179	189
6	243	220
7	-93	-73
-10	287	287
-9	-89	-4
-8	610	-634
-7	-91	137
-6	106	90
-5	-72	56
-4	384	-387
-3	-71	-90
-2	562	577
-1	119	62
H= 7. K= 8		
0	-77	-69
1	-93	84
2	157	149
3	-92	-116
4	-91	17
5	-94	33
6	-95	1
-10	142	85
-9	-94	-68
-8	-91	24
-7	315	314
-6	165	-153
-5	-93	-90
-4	135	-136
-3	119	119
-2	-75	-36
-1	147	-153
H= 8. K= 8		
0	-95	-135
1	-92	28
2	178	136
3	-94	66
4	188	-167
5	-97	9
-9	139	-98
-8	160	-154
-7	-94	45
-6	243	256
-5	-93	41
-4	-94	-109
-3	238	-261
-2	287	311
-1	-95	-53
H= 9. K= 8		
0	-95	63
1	-97	124
2	-96	44
3	228	-222
-8	-97	-3
-7	549	551
-6	-98	-96
-5	204	-189
-4	-95	-36
-3	199	197
-2	-95	22
-1	230	-237
H= 10. K= 8		
0	-103	54
1	-101	75
-6	176	-202
-5	-103	92
-4	-101	65
-3	-100	34
-2	-102	-72
-1	-102	9

L	FO	FC
H=	0, K=	9
1	224	-219
2	-59	-66
3	140	-126
4	-63	66
5	-64	-23
6	-67	49
7	-72	-32
8	-75	-66
9	160	154
10	114	-129
H=	1, K=	9
0	474	466
1	88	-30
2	-60	20
3	523	517
4	119	89
5	371	-378
6	265	-267
7	-78	42
8	112	-108
9	355	-368
10	173	-162
-10	223	-204
-9	303	300
-8	144	-163
-7	-69	-28
-6	-67	17
-5	240	236
-4	495	489
-3	339	-311
-2	394	-394
-1	97	100
H=	2, K=	9
0	108	-139
1	160	-170
2	-62	45
3	241	237
4	110	-140
5	485	-495
6	171	178
7	161	166
8	-82	-49
9	-84	15
-10	304	301
-9	-80	65
-8	472	-471
-7	223	208
-6	-68	-22
-5	461	472
-4	374	-371
-3	380	-348
-2	652	649
-1	-60	-85
H=	3, K=	9
0	186	197
1	-63	9
2	116	95
3	109	102
4	-70	99
5	162	-169
6	-82	38
7	-82	16
8	-83	26
9	-85	46
-10	-83	-25
-9	-81	-50
-8	291	-273
-7	-70	-83
-6	147	135
-5	-66	22
-4	97	-89

L	FO	FC
-3	-63	-29
-2	145	154
-1	-62	46
H=	4, K=	9
0	175	-194
1	415	-411
2	120	110
3	313	335
4	291	-306
5	342	-335
6	232	248
7	219	219
8	-86	-43
-10	221	221
-9	301	318
-8	411	-428
-7	-83	52
-6	-70	75
-5	-68	19
-4	141	-136
-3	235	-233
-2	249	264
-1	-66	65
H=	5, K=	9
0	-69	-113
1	161	139
2	330	338
3	115	-122
4	259	-227
5	-88	93
6	218	233
7	-92	-77
-10	248	269
-9	301	-291
-8	217	-242
-7	454	477
-6	133	-169
-5	-71	7
-4	241	-239
-3	225	234
-2	262	249
-1	386	-376
H=	6, K=	9
0	122	-124
1	185	-190
2	-90	25
3	-89	29
4	-89	-37
5	-90	-65
6	-92	101
-10	-92	0
-9	-89	37
-8	-88	-15
-7	311	316
-6	-89	103
-5	219	-218
-4	-72	-10
-3	-73	74
-2	-72	55
-1	-73	8
H=	7, K=	9
0	198	-211
1	-92	138
2	195	214
3	-93	-113
4	155	-103
5	148	152
-9	156	-170
-8	237	-236
-7	398	383
-6	-90	-101
-5	-92	-151

L	FC	FC
-4	-93	-97
-3	-93	137
-2	357	381
-1	-95	-175
H=	8, K=	9
0	147	174
1	-94	-18
2	-96	-49
3	194	-156
4	-97	72
-8	199	212
-7	259	254
-6	318	-313
-5	-94	-73
-4	-93	17
-3	258	254
-2	157	-192
-1	-95	-124
H=	9, K=	9
0	-97	-36
1	146	81
2	-100	111
-7	-99	32
-6	147	-154
-5	-95	-86
-4	-97	117
-3	-95	14
-2	-95	-21
-1	-96	-14
H=	10, K=	9
-5	-102	14
-4	-104	96
-3	-100	-13
-2	-104	-92
-1	-104	-154
H=	0, K=	10
0	113	154
1	907	-928
2	180	167
3	569	561
4	-65	-11
5	110	-103
6	-68	-45
7	-76	54
8	147	-96
9	349	-355
H=	1, K=	10
0	389	-377
1	155	154
2	220	190
3	99	-75
4	-66	-57
5	-68	58
6	-79	-16
7	-77	-19
8	-78	1
9	-81	-22
-10	337	342
-9	-79	1
-8	-76	-124
-7	-76	28
-6	127	-115
-5	138	135
-4	442	-447
-3	174	-174
-2	365	367
-1	-62	71
H=	2, K=	10

L	FO	FC
0	134	-128
1	308	-295
2	124	89
3	212	217
4	-69	63
5	368	-378
6	140	-143
7	-80	21
8	-84	47
9	175	-155
-10	-85	-109
-9	-80	77
-8	-80	7
-7	-81	-44
-6	-68	31
-5	185	186
-4	162	166
-3	280	-282
-2	171	-178
-1	292	277
H=	3, K=	10
0	588	-580
1	-67	35
2	599	614
3	239	-243
4	429	-424
5	-83	-46
6	148	166
7	-83	84
8	-86	-58
-10	217	202
-9	-83	-53
-8	418	-438
-7	-82	14
-6	205	191
-5	114	138
-4	302	-305
-3	-67	40
-2	564	552
-1	225	-205
H=	4, K=	10
0	-69	2
1	252	234
2	-71	-1
3	136	-134
4	-85	7
5	-82	32
6	-83	-116
7	-86	53
-10	-87	-110
-9	361	-359
-8	-82	-11
-7	-82	136
-6	-83	-32
-5	164	164
-4	-70	-60
-3	305	316
-2	100	-49
-1	237	-239
H=	5, K=	10
0	243	-282
1	-73	-27
2	335	332
3	-89	-13
4	214	-193
5	-87	24
6	219	198
7	-91	17
-9	201	198
-8	-88	-168
-7	-86	-100
-6	-86	84
-5	-88	-49
-4	179	-184

```
  L    FO     FC

 -3   -71    -55
 -2   238    245
 -1   141    115

H=    6,  K=   10

  0   -89     47
  1   470    462
  2   -89     -9
  3   333   -350
  4   188    197
  5   -92    157
  6   -92    -53
 -9   176   -205
 -8   -92    140
 -7   318    321
 -6   144   -115
 -5   -87    -21
 -4   -89    -13
 -3   267    278
 -2   -90    -39
 -1   546   -541

H=    7,  K=   10

  0   200    192
  1   -92    -55
  2   -95   -116
  3   -94     22
  4   -95     40
 -8   202    215
 -7   -95    -85
 -6   -92    -53
 -5   -92     45
 -4   -92   -129
 -3   -94    123
 -2   255   -248
 -1   -92     35

H=    8,  K=   10

  0   -94     14
  1   -96    114
  2   -96    -45
  3   180   -179
 -7   171    158
 -6   -95     49
 -5   -96   -136
 -4   -94    -50
 -3   195    201
 -2   -94     66
 -1   138   -162

H=    9,  K=   10

  0   283    249
  1  -100    -57
 -6   356   -329
 -5   -99     65
 -4   -98     37
 -3   -99    -24
 -2   189   -137
 -1   -99     74

H=    0,  K=   11

  1   -65    -76
  2   -65    -39
  3   129    119
  4   -69    102
  5   -76    -57
  6   -75     50
  7   -74      0
  8   -77    -74
  9   160   -185

H=    1,  K=   11

  0   690   -692
  1   363   -361
```

```
  L    FO     FC

  2   352    363
  3   156    162
  4   458   -451
  5   -79      0
  6   290    304
  7   -78    -20
  8   -81    -76
 -9   120    142
 -8   192   -186
 -7   -78   -115
 -6   -78     42
 -5   -68     10
 -4   308   -292
 -3   403   -407
 -2   368    347
 -1   224    213

H=    2,  K=   11

  0   245   -232
  1   607    616
  2   -68     39
  3   247   -225
  4   335   -337
  5   191    193
  6   144    124
  7   -81    -43
  8   222   -197
 -9   380   -372
 -8   184   -242
 -7   132    121
 -6   -80     -4
 -5   316   -317
 -4   121   -164
 -3   388    392
 -2   283    290
 -1   324   -349

H=    3,  K=   11

  0   -69    -54
  1   -69    -12
  2   171    155
  3   110     46
  4   142   -137
  5   -82   -105
  6   121     89
  7   -84    -29
 -9   213   -201
 -8   163    170
 -7   -80    -50
 -6   -80     -9
 -5   -81     14
 -4   -71     58
 -3   108    134
 -2   -70    -67
 -1   -69    -91

H=    4,  K=   11

  0   101    -60
  1   637    646
  2   355    392
  3   265   -296
  4   338   -351
  5   290    298
  6   136    141
  7   214   -186
 -9   187   -219
 -8   238   -257
 -7   212    231
 -6   158    195
 -5   -83     42
 -4   -84      3
 -3   248    240
 -2   160    176
 -1   384   -366

H=    5,  K=   11
```

```
  L    FO     FC

  0   197    190
  1   333    321
  2   410   -409
  3   -87   -112
  4   171    141
  5   175    182
  6   -92   -108
 -9   231   -205
 -8   396    393
 -7   317    330
 -6   184   -163
 -5   -86     94
 -4   261    267
 -3   -88     54
 -2   201   -196
 -1   283   -318

H=    6,  K=   11

  0   -87     29
  1   -90    119
  2   -90     47
  3   -91   -105
  4   -92    -60
  5   -94     53
 -8   222    205
 -7   141   -123
 -6   -88     -2
 -5   -88    -12
 -4   -86     14
 -3   -86    -20
 -2   -89    -56
 -1   -88    -15

H=    7,  K=   11

  0   212    226
  1   -94     77
  2   427   -431
  3   -98   -142
 -7   169    185
 -6   206   -203
 -5   -95   -150
 -4   -92    -42
 -3   156    150
 -2   -94   -166
 -1   270   -277

H=    8,  K=   11

  0   166    146
  1   -99   -104
  2   -99   -129
 -6   354   -368
 -5   -98    102
 -4   -96     42
 -3   212   -182
 -2   -94    -65
 -1   139    126

H=    9,  K=   11

 -3  -101      8
 -2  -101     15

H=    0,  K=   12

  0   389   -388
  1   435    438
  2   319    308
  3   361    374
  4   688   -710
  5   127     78
  6   290    282
  7   -77     81
  8   208   -230

H=    1,  K=   12

  0   218    221
```

```
  L    FO     FC

  1   184    170
  2   158   -136
  3   -79    -17
  4   116    114
  5   -78     26
  6   -79     81
  7   -80    -67
  8   117   -103
 -8   -81    -21
 -7   132    140
 -6   -77     90
 -5   431   -447
 -4   -78    -85
 -3   328    316
 -2   338    326
 -1   108   -112

H=    2,  K=   12

  0   172   -150
  1   315    289
  2   -82      0
  3   187    203
  4   252   -265
  5   -81   -105
  6   411    411
  7   -84    101
 -8   -82     17
 -7   -82   -111
 -6   157    164
 -5   -79    111
 -4   170   -182
 -3   -82    -33
 -2   -70    110
 -1   -68     12

H=    3,  K=   12

  0   511    532
  1   254    237
  2   388   -400
  3   183   -208
  4   273   -266
  5   523    531
  6   -84     -8
  7   222   -227
 -8   191   -182
 -7   335    325
 -6   156    194
 -5   414   -419
 -4   -80     33
 -3   785    810
 -2   267    289
 -1   222   -231

H=    4,  K=   12

  0   -86     63
  1   -87   -133
  2   -86   -123
  3   -85     26
  4   -86     42
  5   -89    -85
  6   -89      2
 -8   348    354
 -7   -87     69
 -6   149   -133
 -5   -85    -61
 -4   349    366
 -3   129   -103
 -2   146   -184
 -1   135   -133

H=    5,  K=   12

  0   -86    -81
  1   188    181
  2   162   -164
  3   -87    -37
  4   -92   -121
```

```
   L      FO      FC

   5     176     166
  -8     -92       0
  -7     -90      31
  -6     -91     158
  -5     176    -168
  -4     -86      18
  -3     205     180
  -2     -87     -49
  -1     -87    -139

 H=      6,  K=   12

   0     236     242
   1     306    -290
   2     170    -192
   3     228     223
   4     -94      99
  -7     -90      80
  -6     212    -224
  -5     139     -77
  -4     288     313
  -3     -90     -77
  -2     650    -676
  -1     188    -212

 H=      7,  K=   12

   0     -96      36
   1     -95     -47
   2     -98     111
  -6     -97     -42
  -5     -94      61
  -4     -95      52
  -3     231    -248
  -2     -93      58
  -1     -95     133

 H=      8,  K=   12

  -4     195     177
  -3     -97      18
  -2     203    -177
  -1     -97      53

 H=      0,  K=   13

   1     171     185
   2     -76     -60
   3     -75     -54
   4     113     -58
   5     -77      33
   6     -77      -7
   7     135      88

 H=      1,  K=   13

   0     -78       8
   1     311     321
   2     -78      17
   3     131    -129
   4     353    -365
   5     369     389
   6     151     167
   7     185    -183
  -7     -81      81
  -6     118     109
  -5     415    -418
  -4     272    -272
  -3     184     190
  -2     462     464
  -1     -78      21

 H=      2,  K=   13
```

```
   L      FC      FC

   0     291     289
   1     -81     -86
   2     -79      -1
   3     321    -327
   4     180     146
   5     260     261
   6     264    -274
  -7     136     180
  -6     208    -194
  -5     253    -283
  -4     345     360
  -3     532     542
  -2     137    -100
  -1     -81     -16

 H=      3,  K=   13

   0     -82    -123
   1     -81      33
   2     150    -154
   3     -83     -33
   4     -83      -1
   5     -85     106
  -7     -85     -19
  -6     118    -101
  -5     -82     -17
  -4     -79     -24
  -3     -81     -12
  -2     -81      30
  -1     -82    -106

 H=      4,  K=   13

   0     -85      33
   1     -86     -61
   2     253    -272
   3     -89    -144
   4     -89      58
   5     379     376
  -7     -88      35
  -6     -89     -71
  -5     154    -177
  -4     383     408
  -3     198     206
  -2     205    -172
  -1     284    -292

 H=      5,  K=   13

   0     -88      91
   1     173    -149
   2     -88     -21
   3     -91      12
   4     184     214
  -6     -91    -158
  -5     187     177
  -4     203     192
  -3     279    -271
  -2     469    -450
  -1     -88       7

 H=      6,  K=   13

   0     -96      90
   1     -96      89
   2     -94     -10
  -5     -94     102
  -4     -94      39
  -3     -92      19
  -2     -94     -57
  -1     131     -48
```

```
   L      FC      FC

 H=      7,  K=   13

   0     264     267
  -4     185     208
  -3     317    -298
  -2     253    -274
  -1     -99      79

 H=      0,  K=   14

   0     172    -196
   1     214     220
   2     191     219
   3     194    -187
   4     -78     -28
   5     298     299
   6     -81     -56

 H=      1,  K=   14

   0     -78      16
   1     -78     -79
   2     -78       4
   3     -78     -60
   4     -79      15
   5     -80     -28
  -6     230    -209
  -5     126      64
  -4     168     169
  -3     188     204
  -2     263    -291
  -1     -77     -69

 H=      2,  K=   14

   0     -80      39
   1     -80      -6
   2     -80      42
   3     255    -238
   4     136    -145
   5     179     162
  -6     136    -126
  -5     -82     -87
  -4     -80     -43
  -3     -82      91
  -2     214     207
  -1     -78      -4

 H=      3,  K=   14

   0     141     157
   1     120      63
   2     162    -173
   3     146    -118
   4     139     156
  -6     352    -354
  -5     -83      -4
  -4     346     350
  -3     -84      -9
  -2     199    -184
  -1     154    -159

 H=      4,  K=   14

   0     -88     -11
   1     -88      -5
   2     -88      10
   3     -90      28
  -5     193     190
  -4     178     -99
  -3     -89    -114
  -2     -87     -58
  -1     175     168
```

```
   L      FO      FC

 H=      5,  K=   14

   0     -90      56
   1     -90      34
   2     -91     -60
  -4     -91      77
  -3     -89     -31
  -2     -91    -102
  -1     147    -167

 H=      6,  K=   14

  -2     -96      27
  -1     205     194

 H=      0,  K=   15

   1     -79      -5
   2     126     106
   3     -80      56
   4     -81      93

 H=      1,  K=   15

   0     251     268
   1     267     272
   2     119    -126
   3     170    -162
   4     174     153
  -4     141     121
  -3     217     221
  -2     175    -179
  -1     140    -187

 H=      2,  K=   15

   0     226     219
   1     283    -266
   2     127     -98
   3     135     128
  -4     -84      52
  -3     136    -111
  -2     216    -224
  -1     -83     110

 H=      3,  K=   15

   0     -85      51
   1     -85       2
   2     -87     -60
  -4     162      57
  -3     -86      82
  -2     -85     -55
  -1     -86     121

 H=      4,  K=   15

   0     143     113
  -3     131    -130
  -2     165    -155
  -1     166     197

 H=      0,  K=   16

   0     244     230
   1     -80       7

 H=      1,  K=   16

   0     -82      35
```

FIGURE 10

$[M(DAPSC)(H_2O)_2]^{++}$ (M=Mn, Ni) Complex Ions

The atomic numbering scheme and thermal ellipsoids for the Ni(II) complex are illustrated. The Mn(II) complex is essentially identical except for the metal ion. Hydrogen atoms are omitted for clarity.

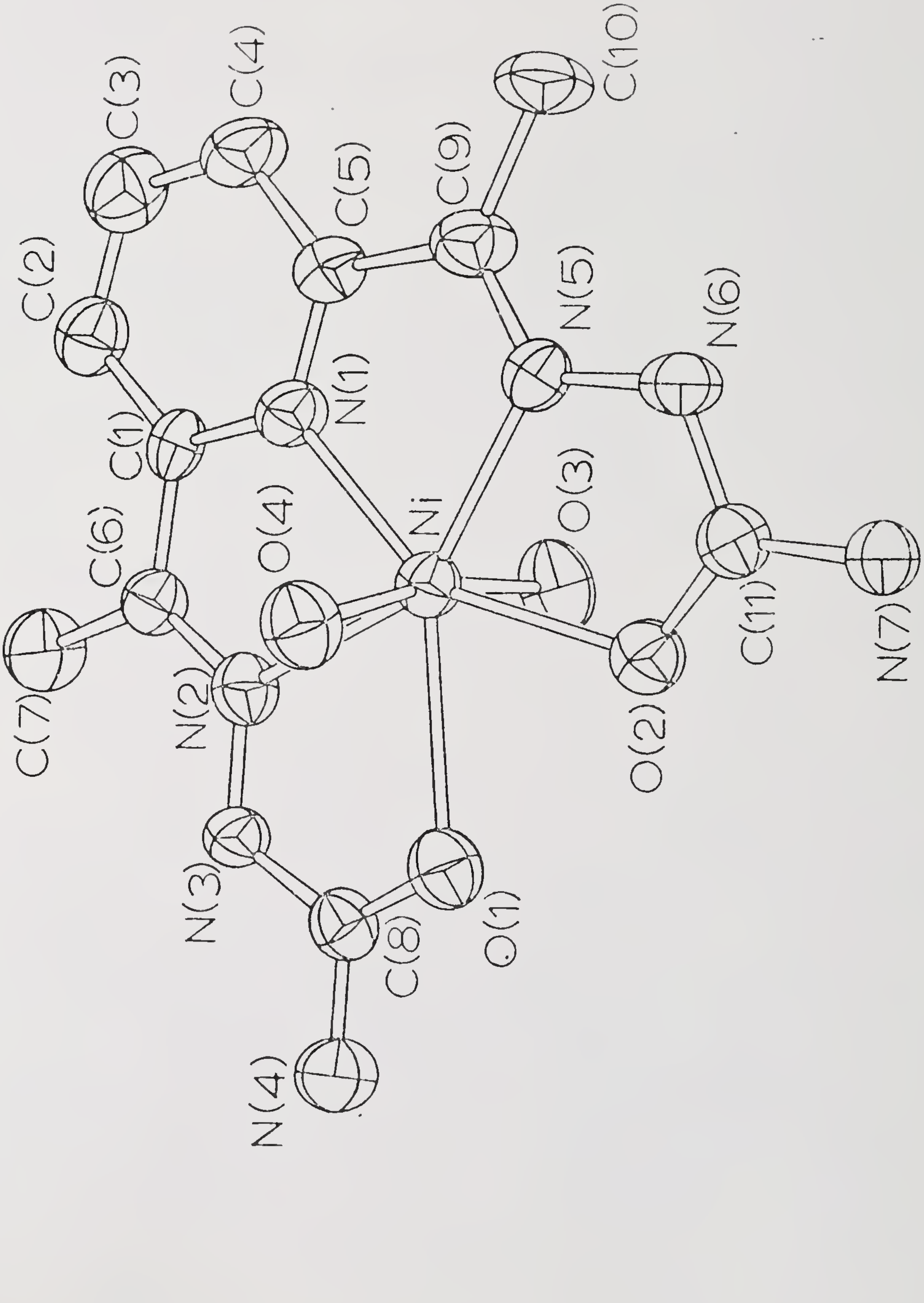
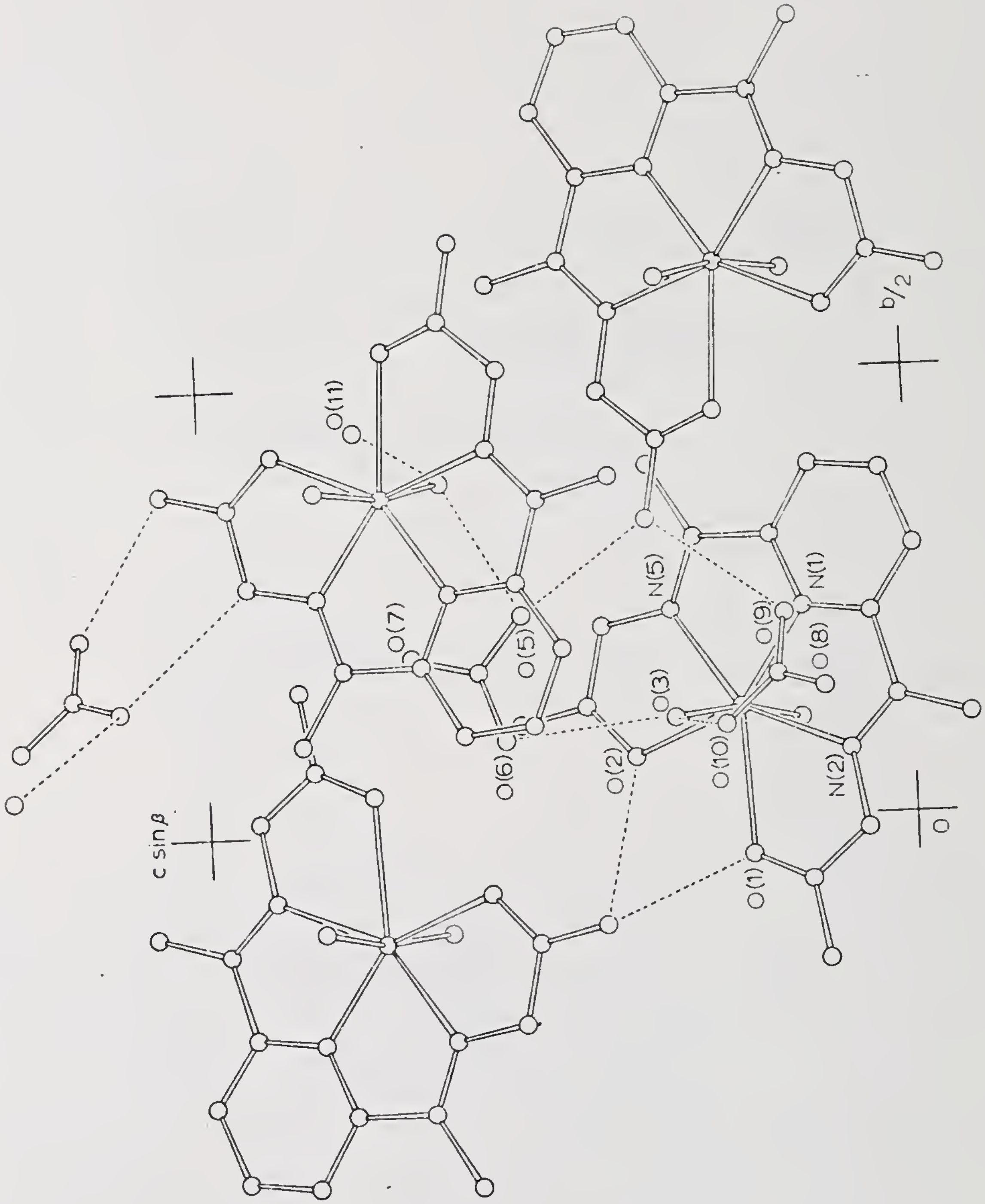

C(10)
C(4)
C(3)
C(5)
C(9)
C(2)
N(5)
N(6)
N(1)
C(1)
O(3)
Ni
O(4)
C(6)
C(11)
N(7)
C(7)
N(2)
O(2)
N(3)
C(8)
O(1)
N(4)

FIGURE 11

A PACKING DIAGRAM FOR $[M(DAPSC)(H_2O)_2](NO_3)_2 \cdot H_2O$

The Ni(II) coordinates were used for this projection along the a axis. The Mn(II) compound is essentially identical. Some atomic labels and hydrogen atoms are omitted for clarity. Dotted lines represent hydrogen bonds listed in Table 25.


O(11)
O(7)
O(5)
O(6)
O(2)
O(3)
N(5)
O(10)
O(9)
N(1)
O(8)
N(2)
O(1)
c sinβ
b/2
0

possessed a two-fold axis. Therefore, the space group $P_{2/c}$ was chosen, requiring the copper atom coordinates to be 0, Y, ¼. The corresponding translation of the trial structure to the proper position was made. The model was refined by three least-squares cycles with isotropic thermal parameters. A difference Fourier synthesis revealed a large peak situated on the two-fold axis. This peak was assigned to a water of hydration. Three additional cycles of least-squares refinement reduced R to 0.063. A difference Fourier synthesis sufficed to locate all hydrogen atoms in the structure. The hydrogen atoms were assigned isotropic thermal parameters one unit larger than the refined isotropic thermal parameters of the bonded atoms. Three least-squares cycles holding the hydrogen atom parameters constant reduced R to 0.056. All parameter shifts were less than one-tenth of their estimated standard deviations and refinement was terminated.

Results for $[Cu(DAPSC)(H_2O)_2](NO_3)_2 \cdot H_2O$

The final positional and thermal parameters for the non-hydrogen atoms are tabulated in Table 28. Probable positional parameters and bond distances for the hydrogen atoms are listed in Table 29. Intramolecular bond distances and angles and short intermolecular contacts appear in Table 30. Least-squares planes and deviations are in Table 31. Observed and calculated structure factors are in Table 32. An ORTEP[58] drawing of the complex ion and the numbering

Table 28

FINAL POSITIONAL AND THERMAL PARAMETERS (x 10^4) FOR THE NON-HYDROGEN ATOMS OF $[Cu(DAPSC)(H_2O)_2](NO_3)_2 \cdot H_2O$

ATOM	X	Y	Z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Cu	0000*	2204(1)	2500*	42(1)	22(1)	133(2)	0	38(2)	0
O1	1426(4)	945(3)	3623(7)	59(4)	32(2)	329(13)	0(5)	28(11)	4(9)
O2	379(3)	2137(3)	-28(5)	71(3)	32(2)	186(8)	3(5)	83(9)	-24(8)
N1	0000*	3830(4)	2500*	75(7)	21(3)	181(17)	0	65(18)	0
N2	1946(3)	2772(3)	3903(6)	51(4)	35(2)	183(11)	-6(6)	24(10)	-8(10)
N3	2878(4)	2120(4)	4549(7)	44(4)	43(3)	278(13)	4(7)	-2(12)	10(12)
N4	3480(5)	544(4)	4865(10)	81(6)	49(4)	408(19)	49(7)	22(17)	5(13)
C1	1076(5)	4292(4)	3267(8)	74(6)	27(3)	149(13)	-26(7)	58(14)	-25(10)
C2	1106(6)	5290(4)	3295(9)	105(7)	30(3)	195(15)	-39(7)	70(17)	-15(11)
C3	0000*	5775(6)	2500*	178(13)	20(4)	238(25)	0	158(30)	0
C4	2179(6)	3677(4)	4046(9)	63(6)	37(3)	206(16)	-31(7)	40(16)	-7(11)
C5	3468(6)	4097(5)	4940(13)	76(7)	60(5)	405(26)	-43(10)	-4(21)	-46(19)
C6	2523(5)	1167(4)	4318(9)	66(6)	44(4)	204(16)	15(8)	44(16)	15(13)
N5	3530(4)	2214(5)	-316(8)	56(5)	73(4)	296(15)	1(9)	90(13)	4(16)
O3	2778(7)	1557(5)	-269(12)	186(9)	93(4)	710(29)	-63(11)	337(26)	-42(18)
O4	4478(5)	1949(6)	-668(11)	73(5)	214(7)	745(28)	16(11)	178(19)	-174(24)
O5	3222(8)	2989(4)	-110(12)	465(15)	57(4)	705(28)	192(13)	505(32)	65(16)
O6	0000*	649(4)	7500*	114(7)	20(3)	286(17)	0	68(16)	0

* Coordinate determined by space group symmetry

Table 29
FINAL POSITIONAL AND THERMAL PARAMETERS (x 10^3) FOR THE HYDROGEN ATOMS OF $[Cu(DAPSC)(H_2O)_2](NO_3)_2 \cdot H_2O$

ATOM	BONDED TO	DISTANCE,Å	X	Y	Z	B(Å^2)
H1	N4	0.98	332	-15	471	5.5
H2	N4	0.99	431	70	576	5.5
H3	N3	0.98	378	226	497	4.3
H4	C5	1.04	4.5	382	428	5.7
H5	C5	1.12	383	387	653	5.7
H6	C5	1.08	337	482	545	5.7
H7	C2	0.96	188	564	378	4.4
H8	C3	1.09	000*	656	250*	5.0
H9	O2	0.92	122	210	-9	3.8
H10	O2	0.93	10	159	-79	3.8
H11	O3	0.88	59	21	791	4.4

* Coordinates determined by space group symmetry

Table 30

INTRAMOLECULAR BOND DISTANCES AND ANGLES AND SHORT INTERMOLECULAR CONTACTS FOR $[Cu(DAPSC)(H_2O)_2](NO_3)_2 \cdot H_2O$ WITH THEIR ESTIMATED STANDARD DEVIATIONS IN PARENTHESES

(a) Bond Distances (Å)

Cu-O1	2.350(4)	N4-C6	1.342(8)
Cu-O2	1.922(3)	C1-C2	1.389(8)
Cu-N1	2.265(6)	C1-C4	1.472(8)
Cu-N2	2.258(4)	C2-C3	1.379(8)
O1-C6	1.220(8)	C4-C5	1.513(10)
N1-C1	1.334(6)	N5-O3	1.238(9)
N2-N3	1.358(6)	N5-O4	1.187(8)
N2-C4	1.285(7)	N5-O5	1.151(9)
N3-C6	1.382(8)		

(b) Bond Angles (°)

O1-Cu-O2	89.1(1)	Cu-N2-C4	121.7(4)
O1-Cu-N1	138.3(1)	N3-N2-C4	120.8(5)
O1-Cu-N2	68.8(1)	N2-N3-C6	115.9(5)
O1-Cu-O1'	83.5(1)	N1-C1-C2	120.3(5)
O1-Cu-N2'	152.2(2)	N1-C1-C4	115.4(5)
O1-Cu-O2'	86.8(1)	C2-C1-C4	124.2(5)
O2-Cu-N1	92.8(1)	C1-C2-C3	118.0(5)
O1-Cu-N2	90.4(1)	C2-C3-C2'	121.3(5)
O2-Cu-N2'	91.5(1)	N2-C4-C1	114.4(5)
O2-Cu-O2'	174.5(1)	N2-C4-C5	124.0(6)
N1-Cu-N2	69.5(1)	C1-C4-C5	121.6(5)
Cu-O1-C6	116.8(4)	O3-N5-O4	113.6(7)
Cu-N1-C1	118.9(3)	O3-N5-O5	118.1(7)
C1-N1-C1'	122.2(4)	O4-N5-O5	128.2(7)
Cu-N2-N3	117.5(3)		

Table 30 - continued

(c) Short Intermolecular Contacts (Å)

ATOM A	EQUIV.POS.	ATOM B	EQUIV.POS.	DIST.
O2	X,Y,Z	O3	X,Y,Z	2.781(8)
O6	X,Y,Z	O1	-X,-Y,1-Z	2.716(6)
O6	X,Y,Z	O2	X,Y,1+Z	2.661(5)
O4	X,Y,1+Z	N3	1-X,Y,½+Z	2.819(7)
O3	X,Y,1+Z	N4	X,-Y,½+Z	3.022(8)
O4	X,Y,1+Z	N4	1-X,Y,1½-Z	2.922(9)
O4	X,Y,1+Z	O4	1-X,Y,½-Z	3.053(9)

Table 31
LEAST-SQUARES PLANES AND DEVIATIONS FOR $[Cu(DAPSC)(H_2O)_2](NO_3)_2 \cdot H_2O$

The title and equation of the plane are given followed by selected atoms and their deviations (x 10^3 Å). Equations are of the form ax+by+cz=d, where d is the distance (Å) from the origin. Atoms used to define the plane are denoted by an asterisk. Dihedral angles between planes are given in degrees and decimal fractions.

Plane 1. Plane Through the Pyridine Ring.

$-0.4453x + 0.8954z = 1.7068$

Cu	0	C3*	0
O1	70	O1'	-70
N1*	0	N2'	-7
N2	7	C1'*	2
C1*	-2	C2'*	-2
C2*	2		

Plane 2. Plane Through the Planar Pentagonal Donor Set.

$-0.4612x + 0.8873z = 1.7001$

Cu	0	N2*	-31
O1*	42	O1'*	-42
N1*	0	N2'*	31

Dihedral Angle Between Planes 1 and 2 = 1.02

Table 32
OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $[Cu(DAPSC)(H_2O)_2](NO_3)_2 \cdot H_2O$

The structure factors for the reflection (HKL) are listed to the right of the appropriate L value under the corresponding H and K values. FO and FC refer to F_{obs} and F_{calc} respectively.

```
   L    FO     FC

 H=    0,  K=    0

   2   709    721
   4   590    605
   6   142   -142
   8   140    132

 H=    1,  K=    0

   0    -8    256
   2   174   -175
   4   527    537
   6   132   -129
  -8   141    131
  -6   202   -211
  -4    50     41
  -2   -10  -2556

 H=    2,  K=    0

   0    40     46
   2   676   -703
   4   237    249
   6   215   -211
  -8   160    157
  -6    57    -40
  -4   854    910
  -2  1367  -1722

 H=    3,  K=    0

   0  1103   1277
   2   123     74
   4   557    573
   6   131   -132
  -8   104     90
  -6   168   -182
  -4  1272   1392
  -2   227    192

 H=    4,  K=    0

   0   466    463
   2   543   -541
   4   335    326
   6   200   -196
  -8    82     93
  -6   553   -561
  -4   512    504
  -2   292   -282

 H=    5,  K=    0

   0   401    415
   2   475   -462
   4   314    311
   6   222   -208
  -8   238    232
  -6   410   -400
  -4   127    134
  -2   616   -617

 H=    6,  K=    0

   0   636    631
   2   357   -359
   4   360    360
   6   136   -142
  -8   238    238
  -6   158   -151
  -4   386    387
  -2   172   -165

 H=    7,  K=    0

   0   391    410
   2   439   -435
   4   209    215
  -6   173   -181

   L    FO     FC

  -4   168    170
  -2   502   -497

 H=    8,  K=    0

   0   394    378
   2   342   -363
   4   188    179
  -6   159   -157
  -4   268    271
  -2   345   -360

 H=    9,  K=    0

   0   404    425
   2   197   -205
   4   137    130
  -6   220   -211
  -4   137    150
  -2   355   -357

 H=   10,  K=    0

   0    68    100
   2   288   -272
  -6   149   -155
  -4   143    150
  -2   488   -483

 H=   11,  K=    0

   0   283    259
   2    77    -76
  -6   127   -130
  -4   262    250
  -2   155   -186

 H=   12,  K=    0

   0    64     57
  -4   121    122
  -2   277   -281

 H=    0,  K=    1

   0    83    260
   1   704   -773
   2   396    401
   3   203    211
   4   159    152
   5   196   -197
   6    63    -64
   7   175    181
   8    45     32

 H=    1,  K=    1

   0   227   -226
   1   588   -598
   2    27     36
   3    68    -50
   4   178    185
   5   350   -355
   6    31    -25
   7   119    113
  -8    48     40
  -7   194   -180
  -6    82    -82
  -5    61     65
  -4    87    -90
  -3   515   -516
  -2   -13    -28
  -1   823    892

 H=    2,  K=    1

   0    68    -68
   1   199    177
   2   242   -245
   3   489    493

   L    FO     FC

   4    59     57
   5   256   -253
   6    72    -69
   7    85     96
  -8    66     61
  -7   123   -127
  -6   -17     14
  -5    98    112
  -4    44    -29
  -3   859   -874
  -2   145    140
  -1   566    495

 H=    3,  K=    1

   0   286    255
   1   685   -652
   2    42    -45
   3   315    303
   4   139    124
   5   196   -211
   6    53    -50
   7   105    100
  -8    30     28
  -7   105   -114
  -6    62     56
  -5   354    329
  -4    53     30
  -3   713   -700
  -2   174    152
  -1   314   -275

 H=    4,  K=    1

   0   256    264
   1   642   -636
   2    63    -46
   3   177    192
   4   154    150
   5   253   -236
   6   -18     18
   7    76     79
  -8   -19    -14
  -7   200   -195
  -6    36     25
  -5   319    323
  -4    40    -40
  -3   359   -343
  -2    44    -41
  -1   103     83

 H=    5,  K=    1

   0    37     29
   1   588   -574
   2   200   -193
   3   217    202
   4    66     51
   5   176   -183
   6    68     66
  -8   -19    -21
  -7   282   -278
  -6    28     27
  -5   140    142
  -4    24     15
  -3   299   -283
  -2   187   -178
  -1   194    203

 H=    6,  K=    1

   0   135    131
   1   374   -362
   2   183   -166
   3   148    161
   4    81    -74
   5   206   -191
   6    45     44
  -8    32    -22
  -7   214   -212

   L    FC     FC

  -6   -17      6
  -5    25     15
  -4   103    108
  -3   412   -416
  -2    57    -60
  -1   398    386

 H=    7,  K=    1

   0   246    239
   1   402   -405
   2    32     33
   3   157    144
   4    96    -93
   5   196   -195
  -7    76    -94
  -6    48    -51
  -5   158    149
  -4    57     55
  -3   440   -448
  -2    66    -53
  -1   123    114

 H=    8,  K=    1

   0    77     58
   1   254   -259
   2   115    115
   3   176    182
   4   -17    -16
   5   117   -115
  -7   143   -135
  -6    53    -53
  -5   150    165
  -4    53     47
  -3   275   -280
  -2   133   -137
  -1   285    275

 H=    9,  K=    1

   0    95    -83
   1   314   -294
   2    63     73
   3   137    140
   4    50     53
  -7   146   -155
  -6    57    -50
  -5   106    106
  -4    25     29
  -3   372   -360
  -2   150   -132
  -1    63     88

 H=   10,  K=    1

   0   131   -139
   1   243   -250
   2    61    -53
   3    45     39
  -6   -19    -27
  -5   173    168
  -4    78     69
  -3   123   -143
  -2   -17    -12
  -1   234    221

 H=   11,  K=    1

   0    30     13
   1    77    -86
   2    54    -60
  -6    41    -39
  -5    84     91
  -4    47     34
  -3   210   -218
  -2   114    109
  -1   205    201
  L    FO     FC

H=  12, K=     1

  0   -18     35
  1   122   -120
 -5   100    115
 -4    67    -68
 -3   201   -135
 -2   -18      4
 -1    81     91

H=   0, K=     2

  0   -10  -1075
  1    47    -47
  2   499   -484
  3    90    125
  4   393   -414
  5    40    -43
  6   203    197
  7    27     20

H=   1, K=     2

  0    36    -56
  1   242   -254
  2    45    -39
  3    58    -48
  4   567   -571
  5    45    -59
  6   121    137
  7    40     27
 -8   157   -151
 -7    49    -57
 -6   167    176
 -5    45     40
 -4   132   -114
 -3    42    -45
 -2   290    294
 -1   -12     27

H=   2, K=     2

  0   193   -169
  1    90     68
  2   526    533
  3    29     59
  4   341   -366
  5    33    -21
  6   130    138
  7    76     78
 -8   154   -155
 -7    56    -65
 -6    53     48
 -5    30    -15
 -4   278   -293
 -3   200   -226
 -2    64    -49
 -1   105     86

H=   3, K=     2

  0   636   -629
  1   157   -164
  2   385    381
  3    67    -64
  4   352   -345
  5   128   -135
  6    72     67
  7    49     45
 -8    93    -96
 -7    36    -37
 -6    45     62
 -5   -16     36
 -4   337   -311
 -3   129   -120
 -2   151   -105
 -1   100    -48

H=   4, K=     2
```

```
  L    FO     FC

  0   872   -846
  1    89     73
  2   307    314
  3    80     83
  4   215   -224
  5   171   -166
  6   -17     17
 -8    52    -64
 -7    37    -34
 -6   133    138
 -5   -15     28
 -4   160   -161
 -3   150   -151
 -2    29     49
 -1   -12     10

H=   5, K=     2

  0   484   -487
  1   148   -158
  2   211    221
  3   211    213
  4   100    -96
  5   -17     -9
  6    77     75
 -8    83    -86
 -7    45    -47
 -6    92    100
 -5   -16     11
 -4    71   -100
 -3   202   -213
 -2   608    578
 -1   257   -236

H=   6, K=     2

  0   274   -287
  1   294   -267
  2   196    193
  3    58     71
  4    62    -58
  5    54     42
  6   123    124
 -8    56    -66
 -7    48    -49
 -6    81     91
 -5    37     50
 -4   296   -295
 -3    43    -12
 -2   434    432
 -1    62     -3

H=   7, K=     2

  0   275   -275
  1   246   -271
  2    27      2
  3    98    -97
  4   174   -193
  5   -18    -14
 -7    46    -47
 -6   132    145
 -5    53     40
 -4   287   -285
 -3   -16    -57
 -2   333    340
 -1    89     49

H=   8, K=     2

  0    37    -14
  1   -17     -4
  2   184    190
  3    74    -63
  4   159   -152
  5    58    -58
 -7    80    -69
 -6   179    181
 -5    33     -7
```

```
  L    FO     FC

 -4   292   -277
 -3    66    -52
 -2   240    247
 -1   227    244

H=   9, K=     2

  0    80    -76
  1    57     61
  2   240    251
  3    33     29
  4    50    -57
 -7    40    -48
 -6   234    228
 -5    34    -26
 -4   106   -119
 -3   231   -227
 -2   172    172
 -1   -17     15

H=  10, K=     2

  0   133   -155
  1   -18    -21
  2   168    159
  3    45     47
 -6   149    157
 -5    80     78
 -4    89    -95
 -3    87    -99
 -2   139    123
 -1    51    -58

H=  11, K=     2

  0   209   -195
  1    45    -43
  2    72     76
 -6   113    119
 -5    76     70
 -4    51    -48
 -3   -17    -17
 -2   107    130
 -1    48    -31

H=  12, K=     2

  0   -18    -18
  1    75    -94
 -4   -18    -12
 -3    40     21
 -2   261    261
 -1   -17      8

H=   0, K=     3

  0   797   -806
  1   264    274
  2   117   -128
  3   568   -562
  4   214   -229
  5   227    218
  6   -17     -2
  7   162   -165

H=   1, K=     3

  0   352   -323
  1  1002   1096
  2   -12     -8
  3   195   -200
  4   203   -190
  5   341    345
  6    78    -66
  7   113   -115
 -8   -19    -15
 -7   171    156
 -6    55     65
 -5   233   -230
 -4   172   -159
```

```
  L    FO     FC

 -3   511    506
 -2   267    248
 -1   226    193

H=   2, K=     3

  0   367   -320
  1   205    211
  2   127    119
  3   582   -583
  4    66     42
  5   216    206
  6    53     52
  7   103   -100
 -8    49    -60
 -7   146    147
 -6    58     54
 -5   272   -272
 -4   249   -243
 -3   113    123
 -2    64     59
 -1   842   -828

H=   3, K=     3

  0   243   -207
  1   944    941
  2   146   -128
  3   277   -279
  4    61    -50
  5   201    202
  6   126    123
  7    51    -47
 -8    64    -65
 -7   193    189
 -6    67     74
 -5    84    -87
 -4   218   -206
 -3   480    464
 -2   165    177
 -1   174   -173

H=   4, K=     3

  0   282   -295
  1   742    732
  2   218   -200
  3   123   -118
  4   233   -226
  5   203    189
  6    54     71
 -8    59    -61
 -7   144    142
 -6    94     89
 -5    79    -95
 -4   236   -235
 -3   523    505
 -2    46    -75
 -1   394   -365

H=   5, K=     3

  0   178    175
  1   307    285
  2   119    119
  3   258   -256
  4   204   -202
  5    43     41
  6   -18     29
 -8    63    -65
 -7   106    112
 -6    90    100
 -5   207   -198
 -4   110    -82
 -3   336    314
 -2   208    232
 -1   635   -647
```

L	FC	FC
H= 6, K= 3		
0	85	45
1	431	439
2	355	350
3	30	28
4	-17	-39
5	206	192
6	46	50
-7	158	154
-6	100	91
-5	84	-85
-4	122	-137
-3	562	584
-2	-14	-30
-1	241	-201
H= 7, K= 3		
0	383	-388
1	238	230
2	65	69
3	65	-56
4	57	-60
5	237	234
-7	118	120
-6	92	89
-5	199	-199
-4	38	-46
-3	423	410
-2	108	-101
-1	154	-160
H= 8, K= 3		
0	173	-155
1	-17	-6
2	51	67
3	304	-315
4	84	-74
-7	132	135
-6	51	61
-5	198	-194
-4	-17	27
-3	221	216
-2	173	195
-1	272	-271
H= 9, K= 3		
0	-17	-44
1	367	371
2	104	95
3	129	-125
4	54	-55
-7	141	142
-6	60	44
-5	117	-108
-4	27	2
-3	328	336
-2	296	263
-1	132	133
H= 10, K= 3		
0	-17	-11
1	310	309
2	114	113
3	-18	-16
-6	-18	20
-5	168	-170
-4	138	-134
-3	30	33
-2	122	134
-1	149	-152
H= 11, K= 3		
0	119	-112

L	FC	FC
1	40	45
2	53	59
-5	67	-65
-4	97	-101
-3	53	55
-2	-17	19
-1	303	-306
H= 12, K= 3		
0	-18	-22
-4	-18	14
-3	208	211
-2	140	140
-1	77	-89
H= 0, K= 4		
0	333	291
1	146	141
2	86	-75
3	515	-537
4	291	306
5	190	189
6	37	-26
7	55	-58
H= 1, K= 4		
0	270	250
1	633	651
2	229	-237
3	345	-350
4	196	192
5	137	146
6	35	-43
7	50	-51
-7	96	91
-6	75	-85
-5	267	-270
-4	274	266
-3	268	262
-2	93	-93
-1	104	-115
H= 2, K= 4		
0	516	480
1	616	605
2	178	-183
3	270	-286
4	97	114
5	93	88
6	108	-106
7	85	-88
-8	68	64
-7	148	150
-6	95	-100
-5	167	-162
-4	249	244
-3	261	269
-2	67	40
-1	294	-282
H= 3, K= 4		
0	446	453
1	743	722
2	53	49
3	-15	-15
4	232	230
5	152	160
6	40	-46
7	85	-84
-8	73	75
-7	165	158
-6	98	-109
-5	84	-89
-4	165	176
-3	329	324

L	FC	FC
-2	167	-146
-1	312	-304
H= 4, K= 4		
0	143	99
1	166	185
2	176	-185
3	65	-88
4	150	155
5	218	208
6	-17	-12
-8	71	80
-7	119	117
-6	96	-97
-5	79	-85
-4	122	116
-3	364	368
-2	320	-339
-1	577	-572
H= 5, K= 4		
0	149	152
1	259	259
2	199	-200
3	203	-199
4	-17	35
5	121	123
6	91	-89
-7	111	112
-6	54	-58
-5	109	-108
-4	240	255
-3	500	510
-2	156	-128
-1	68	-74
H= 6, K= 4		
0	295	303
1	321	312
2	31	-27
3	104	-111
4	95	92
5	150	143
-7	132	124
-6	121	-128
-5	106	-124
-4	176	170
-3	392	373
-2	54	-58
-1	24	-58
H= 7, K= 4		
0	86	72
1	290	302
2	51	-50
3	101	-96
4	171	175
5	156	153
-7	96	110
-6	126	-128
-5	186	-169
-4	36	28
-3	156	182
-2	275	-290
-1	107	-88
H= 8, K= 4		
0	31	-13
1	160	150
2	196	-192
3	153	-167
4	132	135
-7	144	133
-6	54	-58
-5	49	-61

L	FC	FC
-4	136	147
-3	151	145
-2	185	-166
-1	219	-234
H= 9, K= 4		
0	120	104
1	241	251
2	209	-217
3	112	-106
4	35	47
-6	82	-91
-5	-17	-10
-4	126	121
-3	294	298
-2	54	-65
-1	24	-19
H= 10, K= 4		
0	165	169
1	201	207
2	124	-134
3	41	-41
-6	105	-115
-5	135	-129
-4	47	55
-3	84	93
-2	81	-82
-1	160	-154
H= 11, K= 4		
0	147	156
1	90	71
2	39	-39
-5	68	-74
-4	-17	11
-3	122	129
-2	149	-152
-1	162	-178
H= 12, K= 4		
0	26	31
-4	40	39
-3	142	147
-2	192	-196
-1	79	-71
H= 0, K= 5		
0	701	713
1	103	-117
2	49	-34
3	94	103
4	516	529
5	43	-55
6	102	-91
7	44	51
H= 1, K= 5		
0	310	278
1	127	81
2	444	-436
3	173	166
4	437	437
5	-17	-26
6	46	-52
7	79	77
-7	-18	-34
-6	193	-193
-5	113	110
-4	362	342
-3	22	8
-2	209	-227
-1	341	347

```
   L    FC     FC       L    FO     FC       L    FO     FC       L    FO     FC

                      -5    36     44    H=    0, K=     6
H=    2, K=     5       -4   354    352                             H=    5, K=     6
                      -3    99   -124       0   751   -709
   0   780    753       -2   219   -209       1   327   -314       0   262   -248
   1   322   -297       -1    37     19       2   250    245       1   376   -356
   2   518   -510                             3   361    363       2   245    248
   3    59    -50    H=    7, K=     5       4   129   -133       3   164    161
   4   165    173                             5   216   -215       4   108   -107
   5   128   -128        0   175    162       6    58     55       5   174   -177
   6   114   -116        1    57    -75       7   101    103       6    72     69
   7    43     47        2   170   -175                            -7   159   -160
  -7    68    -72        3    52     46    H=    1, K=     6      -6   126    128
  -6   161   -154        4   175    173                            -5   105     98
  -5    59     35        5   100    -98       0   511   -465      -4   206   -201
  -4   344    361       -7    53    -64       1   219   -230      -3   493   -486
  -3   257   -271       -6   209   -206       2   128    133      -2   -15    -11
  -2    55     53       -5    52     59       3   417    411      -1    91     96
  -1   164   -125       -4   156    162       4   112   -110
                      -3    49    -54       5   143   -150    H=    6, K=     6
H=    3, K=     5       -2   277   -271       6   100     89
                      -1   186    187       7   108    104       0   341   -345
   0   868    837                            -7   117   -115       1   339   -351
   1   102   -123    H=    8, K=     5      -6    81     76       2   105    100
   2   139   -137                            -5   267    262       3   119    127
   3    41     52        0   114    114      -4   129   -125       4   142   -142
   4   272    267        1    73    -68      -3   165   -177       5   189   -180
   5   122   -123        2   246   -249      -2   524    512      -7   152   -149
   6    79    -79        3    81     88      -1   589    574      -6   108    109
  -7    89    -83        4   125    123                            -5   110    125
  -6   119   -132       -7    60    -60    H=    2, K=     6      -4    96    -79
  -5    44     56       -6   138   -139                            -3   402   -404
  -4   242    218       -5   -17     11       0   262   -256      -2    80     75
  -3   160   -163       -4   174    177       1   677   -651      -1   107     94
  -2   252   -262       -3   163   -161       2    81     90
  -1    43     42       -2   195   -183       3   191    199    H=    7, K=     6
                      -1    70     89       4   151   -138
H=    4, K=     5                             5   190   -183       0   111    -94
                   H=    9, K=     5       6   106    108       1   285   -283
   0   521    499                             7    84     92       2   202    209
   1    44    -18        0   201    211      -7   167   -168       3   153    156
   2   200   -193        1   107   -115      -6    41     50       4    51    -47
   3   174    159        2   195   -192      -5   119    125       5   146   -143
   4   190    180        3    83     84      -4   296   -293      -7   119   -128
   5    53    -59       -6   144   -141      -3   518   -504      -6    87     85
   6    90    -92       -5    61     61      -2   474    453      -5   188    190
  -7    54    -63       -4   101    105      -1    34     26      -4   -17    -14
  -6   144   -132       -3   129   -145                            -3   223   -214
  -5    93    103       -2   159   -148    H=    3, K=     6      -2   278    296
  -4   198    213       -1   -16     12                            -1   164    166
  -3    78    -77                             0   221   -207
  -2   471   -447    H=   10, K=     5       1   643   -627    H=    8, K=     6
  -1   142    135                             2    62     49
                       0   134    129       3    83     77       0   184   -190
H=    5, K=     5        1   124   -126       4   238   -242       1   237   -234
                       2   157   -166       5   188   -201       2    84     86
   0   290    294       -6   119   -122       6    67     60       3   143    154
   1   249   -223       -5    77     90      -7   173   -166       4    78    -73
   2   174   -161       -4    79     71      -6   108    100      -6    42     37
   3    73     77       -3    42    -53      -5   150    150      -5    96     93
   4   147    148       -2   213   -229      -4   369   -361      -4   117   -128
   5    43    -48       -1    61     67      -3   376   -368      -3   226   -221
   6   139   -125                            -2   211    202      -2   154    140
  -7    74    -82    H=   11, K=     5      -1   217    202      -1   193    198
  -6    84    -91
  -5    53     49        0   162    168    H=    4, K=     6    H=    9, K=     6
  -4   311    309        1    80    -77
  -3   161   -161       -5    37     50       0    48     54       0   126   -133
  -2   489   -468       -4    95     93       1   205   -203       1   241   -262
  -1   100    -35       -3    59    -52       2   322    309       2    64     59
                      -2   162   -157       3   185    185       3    93     82
H=    6, K=     5       -1    88    100       4   145   -143      -6    54     60
                                            5   198   -189      -5    79     72
   0   248    237    H=   12, K=     5       6    75     72      -4   120   -111
   1   233   -249                            -7   136   -139      -3   256   -277
   2   165   -156        0    38     42      -6   198    188      -2   132    139
   3   -17     -1       -4    70     65      -5   170    172      -1   106     92
   4   189    183       -3    69    -76      -4   173   -170
   5    82    -92       -2   205   -213      -3   267   -258    H=   10, K=     6
  -7    79    -81       -1    85     92      -2   289    274
  -6   144   -148                            -1   542    538       0    55    -39
```

```
   L    FO     FC

   1   189   -187
   2   102    110
  -5   123    135
  -4    81    -73
  -3   142   -135
  -2   135    152
  -1   169    185

H=   11,  K=    6

   0    77    -82
   1    70    -63
  -4    78    -89
  -3   171   -170
  -2    87     78
  -1   152    165

H=   12,  K=    6

  -3   129   -150
  -2    70     63
  -1    81     73

H=    0,  K=    7

   0   649   -653
   1   460    472
   2   188    173
   3    36     36
   4   359   -376
   5    30     35
   6   141    133
   7    57    -52

H=    1,  K=    7

   0   492   -449
   1   -13    -13
   2   266    274
   3    32    -26
   4   388   -386
   5    70     69
   6    94    100
   7    28    -32
  -7    40     40
  -6   164    159
  -5   -17     11
  -4   296   -299
  -3   174    177
  -2   300    303
  -1   649   -663

H=    2,  K=    7

   0   645   -644
   1   -14      2
   2   299    283
   3    52    -69
   4   271   -278
   5    69     65
   6   145    141
  -7   -19     11
  -6    98    100
  -5    58    -45
  -4   372   -371
  -3   409    408
  -2   127    122
  -1   200   -185

H=    3,  K=    7

   0   547   -534
   1   -14      8
   2   210    213
   3   125   -127
   4   321   -315
   5    58     47
   6   124    121
  -7   -18     14
  -6   111    117
```

```
   L    FO     FC

  -5   168   -167
  -4   298   -288
  -3   320    312
  -2   291    265
  -1   -14     15

H=    4,  K=    7

   0   342   -329
   1   149    162
   2   320    320
   3    72    -66
   4   267   -269
   5    98     92
   6    97     99
  -7    59     57
  -6    39    144
  -5   240   -222
  -4   200   -213
  -3    29     33
  -2   419    405
  -1    25     11

H=    5,  K=    7

   0   392   -403
   1    56     57
   2   289    281
   3   128   -130
   4   222   -220
   5    81     83
  -7   119    112
  -6    92     91
  -5    93    -89
  -4   324   -322
  -3    37    -34
  -2   269    255
  -1   145   -148

H=    6,  K=    7

   0   359   -350
   1   138    132
   2   275    284
   3   127   -137
   4   172   -163
   5    34     35
  -7    82     78
  -6   142    145
  -5   -17      5
  -4   279   -268
  -3    92     94
  -2   233    247
  -1    54    -56

H=    7,  K=    7

   0   269   -270
   1   149    174
   2   239    246
   3    63    -62
   4   101    -95
  -7   -19     13
  -6   193    186
  -5    31    -42
  -4   137   -151
  -3    39     49
  -2   349    350
  -1   118    -99

H=    8,  K=    7

   0   236   -260
   1   108    103
   2   176    156
   3    35    -41
   4    65    -72
  -6   145    141
  -5    50    -55
  -4   203   -209
```

```
   L    FO     FC

  -3    61     53
  -2   264    249
  -1   116   -142

H=    9,  K=    7

   0   176   -165
   1    35     49
   2   113    114
   3   -19    -28
  -6   154    158
  -5    46    -41
  -4   141   -134
  -3    52     64
  -2   258    275
  -1   150   -143

H=   10,  K=    7

   0    72    -55
   1    37     29
   2   107    120
  -5    39    -33
  -4   137   -134
  -3   116    109
  -2   226    242
  -1    56    -66

H=   11,  K=    7

   0    76    -86
  -4   122   -131
  -3    71     68
  -2   140    120
  -1    35    -34

H=    0,  K=    8

   0   204   -205
   1   321    327
   2    82    -80
   3   230   -223
   4   117   -113
   5   228    225
   6    97    -93
   7   126   -123

H=    1,  K=    8

   0    48     33
   1   253    252
   2   170    155
   3   279   -267
   4    76     71
   5   227    231
   6    56    -53
  -7   159    159
  -6   -18    -14
  -5   176.  -171
  -4    74    -60
  -3   202    211
  -2    49     59
  -1   415   -394

H=    2,  K=    8

   0   190   -160
   1   320    285
   2    23     -1
   3   327   -333
   4   121    112
   5   152    144
   6   -18     14
  -7   147    151
  -6    45     32
  -5   115   -117
  -4   -17    -29
  -3   331    333
  -2    59    -38
  -1   239   -245
```

```
   L    FO     FC

H=    3,  K=    8

   0   180   -184
   1   578    599
   2   251   -233
   3   131   -113
   4    53    -36
   5   215    211
   6   -18     -4
  -7   142    136
  -6   -17      3
  -5    75    -88
  -4   -17    -29
  -3   394    395
  -2    28     -4
  -1    71    -30

H=    4,  K=    8

   0   154    161
   1   365    347
   2    26    -27
   3   126   -131
   4   -17    -21
   5   263    244
  -7    94    106
  -6   -18    -12
  -5   145   -149
  -4    35     -2
  -3   252    229
  -2   119    142
  -1   325   -333

H=    5,  K=    8

   0   144    127
   1   162    160
   2    53     50
   3   346   -324
   4   -18     13
   5    90     89
  -7   109    121
  -6   -17    -14
  -5   134   -118
  -4    68    -75
  -3   267    276
  -2   -16    -42
  -1   366   -345

H=    6,  K=    8

   0    83    -63
   1   464    474
   2   -17    -11
   3   125   -116
   4   -18      1
   5    73     72
  -6   -18     16
  -5    55    -67
  -4    54    -48
  -3   467    457
  -2   202   -184
  -1    26     14

H=    7,  K=    8

   0   -17    -13
   1   395    388
   2    27     -8
   3   -17      5
   4   -18     -7
  -6    48     33
  -5   191   -193
  -4   129    118
  -3   215    207
  -2   -17      2
  -1   161   -174
```

```
   L    FO     FC

H=    8,  K=    8

   0    64     32
   1    88     73
   2    40     15
   3    81    -76
  -6    42    -44
  -5   153   -140
  -4    64     52
  -3   114    131
  -2    56     31
  -1   381   -369

H=    9,  K=    8

   0    29    -11
   1   113    129
   2   -17     11
  -5    35    -39
  -4   -18     -0
  -3   315    324
  -2    46    -20
  -1   105    -79

H=   10,  K=    8

   0    30     17
   1   119    108
  -5   104   -124
  -4   -18     11
  -3   219    197
  -2   -18     12
  -1    41    -50

H=   11,  K=    8

   0   -19    -29
  -3    79     82
  -2   -18     -6
  -1    86    -89

H=    0,  K=    9

   0   342    353
   1    96    101
   2   205   -193
   3   -16      7
   4   208    224
   5    99    -85
   6    52    -58

H=    1,  K=    9

   0   432    408
   1    58     57
   2    96   -110
   3   119    120
   4   225    229
   5   125   -114
   6   -18      9
  -6    89   -102
  -5   -17     19
  -4   215    226
  -3    28     45
  -2   179   -193
  -1   138   -118

H=    2,  K=    9

   0   357    376
   1    74    -73
   2   152   -138
   3   200    200
   4    89     96
   5    30    -31
   6    60    -60
  -6    67    -77
  -5   -17     -1
  -4   267    278
```

```
   L    FO     FC

  -3   130    119
  -2   159   -145
  -1    53    -57

H=    3,  K=    9

   0   294    271
   1   126   -143
   2    60    -62
   3   173    171
   4    97     93
   5    49     58
   6   135   -131
  -6   103   -108
  -5    30    -36
  -4   239    236
  -3   103     98
  -2   203   -217
  -1    78     66

H=    4,  K=    9

   0   188    188
   1   219   -214
   2   -16      0
   3   -16    -10
   4   227    228
   5    55     54
  -6   133   -133
  -5   -17    -29
  -4   176    199
  -3    75     62
  -2   235   -224
  -1   153    158

H=    5,  K=    9

   0    69     65
   1   -17    -11
   2   158   -160
   3    42    -55
   4   197    207
   5   -18     24
  -6    89   -104
  -5    32    -21
  -4   221    222
  -3   -17    -15
  -2   154   -147
  -1   282    270

H=    6,  K=    9

   0   124    102
   1    90    115
   2   246   -276
   3   -17    -14
   4   106     99
  -6   123   -127
  -5    29     11
  -4   177    168
  -3   130   -121
  -2    62    -77
  -1   141    150

H=    7,  K=    9

   0   236    255
   1   105    100
   2   169   -166
   3    44     19
   4    63     70
  -6   134   -133
  -5    90     78
  -4    76     82
  -3    88    -98
  -2    79    -72
  -1    31      1

H=    8,  K=    9
```

```
   L    FO     FC

   0   203    216
   1   -17     21
   2    98    -95
   3   -18     14
  -5   107    104
  -4   -18     34
  -3    47    -14
  -2   190   -179
  -1   101    -83

H=    9,  K=    9

   0    87     83
   1   -18     -1
   2    94    -99
  -5    68     63
  -4    54     44
  -3    91     87
  -2   244   -265
  -1   -17    -10

H=   10,  K=    9

   0    60     57
   1    39     31
  -4   140    139
  -3    54     54
  -2   146   -160
  -1    35     21

H=    0,  K=   10

   0   296    301
   1   273   -276
   2    63     61
   3   243    248
   4    68     71
   5   122   -123
   6    29    -19

H=    1,  K=   10

   0   103    116
   1   296   -292
   2    27     37
   3   218    235
   4    89     86
   5    35    -32
   6    29    -21
  -6   -18    -15
  -5   163    164
  -4    28     37
  -3   245   -238
  -2   109   -103
  -1   272    260

H=    2,  K=   10

   0    78     57
   1   302   -302
   2   -17      0
   3   106    113
   4    61     71
   5   -18    -12
  -6   -18      9
  -5   151    141
  -4   100     97
  -3   245   -253
  -2    45    -75
  -1   271    262

H=    3,  K=   10

   0    72     83
   1   322   -335
   2   -17      7
   3    59    -58
   4   111    105
   5   137   -139
  -6   -18      1
```

```
   L    FO     FC

  -5   107    114
  -4   127    135
  -3   303   -303
  -2   -16     15
  -1   176    165

H=    4,  K=   10

   0    35     34
   1    98    -68
   2    56    -66
   3    32     47
   4   114    117
   5   219   -213
  -6    40    -39
  -5   152    146
  -4    65     72
  -3   232   -233
  -2   -17     -9
  -1   239    249

H=    5,  K=   10

   0    39     49
   1    26    -14
   2   127   -122
   3   250    238
   4    64     73
  -6    35    -35
  -5   120    119
  -4    33     33
  -3   227   -241
  -2    39    -36
  -1   146    115

H=    6,  K=   10

   0   137    125
   1   303   -301
   2   108   -124
   3   152    167
   4   -19    -10
  -6   -19    -16
  -5    81     88
  -4    64     61
  -3   259   -248
  -2    28      3
  -1   145   -113

H=    7,  K=   10

   0   131    142
   1   287   -299
   2   -17    -24
   3    81     94
  -5   126    122
  -4   -18     18
  -3   -17    -28
  -2    95    -80
  -1   106    105

H=    8,  K=   10

   0    42     53
   1   159   -170
   2   -18     12
  -5   -19     25
  -4   -18     25
  -3    52    -62
  -2   144   -134
  -1   247    247

H=    9,  K=   10

   0   -18    -17
   1   142   -154
  -4    60     59
  -3   212   -215
  -2    78    -98
  -1   141    142
```

```
   L    FO     FC

H=  10,  K=   10

   0   -18    -20
  -3   183   -175
  -2    54    -39
  -1    94    115

H=   0,  K=   11

   0   253   -277
   1   182   -194
   2    64     46
   3    83     98
   4   357   -354
   5   173   -174
   6    40     52

H=   1,  K=   11

   0   130   -109
   1   134   -153
   2   332    355
   3   155    160
   4   193   -204
   5   202   -206
  -6   167    160
  -5    76     75
  -4   186   -187
  -3   111   -134
  -2   125    133
  -1   204    197

H=   2,  K=   11

   0   285   -307
   1   134   -146
   2   345    342
   3   281    288
   4    65    -78
   5   127   -128
  -6   142    135
  -5    36     44
  -4   138   -137
  -3   184   -179
  -2    92     79
  -1   139    150

H=   3,  K=   11

   0   577   -557
   1   384   -389
   2    31     33
   3   159    156
   4   177   -176
   5   116   -116
  -6    80     79
  -5    63     63
  -4   144   -144
  -3   198   -201
  -2    56     68
  -1   -17     27

H=   4,  K=   11

   0   154   -176
   1   335   -354
   2   140    143
   3    89     88
   4   160   -158
  -6    81     83
  -5    74     81
  -4    54    -62
  -3   107   -115
  -2   417    404
  -1   196    196

H=   5,  K=   11

   0   110   -119
```

```
   L    FO     FC

   1   167   -172
   2   190    187
   3   129    129
   4   122   -130
  -5    46     43
  -4   226   -220
  -3   141   -147
  -2   242    258
  -1   297    307

H=   6,  K=   11

   0   246   -232
   1   200   -214
   2   100    120
   3    39     30
  -5   -18     19
  -4   237   -237
  -3   301   -303
  -2    70     80
  -1   127    125

H=   7,  K=   11

   0   107   -124
   1   179   -163
   2   179    167
   3   -18    -16
  -5   113    113
  -4    79    -55
  -3   232   -219
  -2   190    190
  -1    65     94

H=   8,  K=   11

   0   156   -150
   1    27    -27
   2    79     91
  -4    85    -92
  -3   102   -121
  -2   149    154
  -1   156    136

H=   9,  K=   11

   0   105   -108
  -3   149   -148
  -2   137    145
  -1    28     11

H=   0,  K=   12

   0   338   -342
   1   -17      6
   2    41    -39
   3   219   -229
   4   143   -149
   5   138    140

H=   1,  K=   12

   0   142   -150
   1   198    203
   2   -16     17
   3   230   -239
   4   213   -208
   5   100    100
  -5   165   -167
  -4    51    -58
  -3    97     93
  -2   161    152
  -1    50     47

H=   2,  K=   12

   0    69    -60
   1   298    309
   2   180    181
   3   144   -154
```

```
   L    FO     FC

   4   126   -127
   5   105    110
  -5    98    -95
  -4   144   -144
  -3   -17     -4
  -2   109    120
  -1    97    -93

H=   3,  K=   12

   0   237   -241
   1   221    235
   2   122    127
   3   132   -133
   4    89    -82
  -5   -18      0
  -4   192   -194
  -3    50     58
  -2    43    -33
  -1   242   -247

H=   4,  K=   12

   0   235   -246
   1   194    188
   2    65     63
   3   104   -121
   4    72    -66
  -5   -18      1
  -4    67    -76
  -3   177    190
  -2    75     69
  -1   219   -228

H=   5,  K=   12

   0   130   -127
   1   147    172
   2    60     55
   3    93    -87
  -5    57    -67
  -4    48    -40
  -3   232    235
  -2   188    197
  -1   174   -161

H=   6,  K=   12

   0    92    -85
   1   149    137
   2    40     43
   3    50    -59
  -5   131   -127
  -4   130   -126
  -3   192    189
  -2   131    134
  -1   109   -136

H=   7,  K=   12

   0    38    -46
   1   101     99
   2    54     60
  -4   112   -125
  -3   123    141
  -2   110     94
  -1   138   -123

H=   8,  K=   12

   0    34    -29
   1    61     67
  -3   142    141
  -2    70     71
  -1    72    -77

H=   9,  K=   12

  -1    44    -52
```

```
   L    FO     FC

H=   0,  K=   13

   0   137    159
   1   166    175
   2   110   -120
   3    77    -70
   4   155    149
   5    86     89

H=   1,  K=   13

   0   126    133
   1   111    105
   2   190   -191
   3    91    -95
   4    78     92
  -5    51    -48
  -4   129    134
  -3   132    140
  -2    99   -109
  -1   174   -179

H=   2,  K=   13

   0   180    200
   1   103    119
   2   139   -134
   3   122   -119
   4    80     87
  -5    57    -55
  -4    86     92
  -3   198    209
  -2   106   -108
  -1   102    -81

H=   3,  K=   13

   0   222    213
   1   203    196
   2    57    -73
   3    54    -49
   4   119    118
  -5    99   -106
  -4    65     78
  -3   173    157
  -2   118   -134
  -1   -17    -37

H=   4,  K=   13

   0    76     97
   1   180    175
   2   124   -123
   3   -18     -1
  -4    87     91
  -3    96     99
  -2   207   -193
  -1    88    -83

H=   5,  K=   13

   0   126    119
   1    76     82
   2   128   -123
   3    34    -25
  -4   153    137
  -3   108    115
  -2    93   -114
  -1   136   -117

H=   6,  K=   13

   0   140    137
   1    91     77
   2    88   -100
  -4    88    102
  -3   186    160
  -2    97    -93
  -1   -18    -48
```

```
    L     FO      FC

 H=     7,  K=   13

    0     96     111
    1     58      95
   -3    127     136
   -2    124    -123
   -1    -18       9

 H=     8,  K=   13

   -2     89    -105
   -1     41     -24

 H=     0,  K=   14

    0    316     326
    1    165    -169
    2     63     -72
    3    130     140
    4    163     164

 H=     1,  K=   14

    0    203     222
    1    235    -249
    2     89     -91
    3    -18      16
    4    170     173
   -4    119     126
   -3    194    -194
   -2    177    -183
   -1     89      95
```

```
    L     FO      FC

 H=     2,  K=   14

    0    149     151
    1     45     -25
    2    163    -163
    3    104     100
   -4    170     176
   -3     77     -80
   -2    159    -164
   -1    258     264

 H=     3,  K=   14

    0    235     231
    1     45     -49
    2    104    -117
    3    107     102
   -4    197     195
   -3    165    -167
   -2     63     -72
   -1    125     120

 H=     4,  K=   14

    0    196     212
    1    137    -135
    2    109    -111
   -4    117     122
   -3    157    -165
   -2    126    -114
   -1    -18       5

 H=     5,  K=   14
```

```
    L     FO      FC

    0    149     147
    1     56     -62
    2    117    -123
   -3     46     -28
   -2    154    -163
   -1    127     120

 H=     6,  K=   14

    0    144     143
    1    134    -125
   -3     70     -63
   -2    138    -139
   -1     75      77

 H=     7,  K=   14

   -1    101      90

 H=     0,  K=   15

    0     57     -79
    1    129    -130
    2     47      47
    3     92      88

 H=     1,  K=   15

    0     55     -53
    1    142    -134
    2    -18      12
    3     41      45
   -3    125    -123
   -2     78      85
```

```
    L     FO      FC

   -1    105     114

 H=     2,  K=   15

    0     30       0
    1     90     -86
    2     34      19
   -3    115    -130
   -2     94      89
   -1    129     112

 H=     3,  K=   15

    0    -18       0
    1     86     -92
    2     39      29
   -3    143    -139
   -2     56      41
   -1     63      68

 H=     4,  K=   15

    0    -19     -16
    1    131    -135
   -3    117    -125
   -2    -18      11
   -1     31      31

 H=     5,  K=   15

    0     31     -14
   -2     27      25
```

FIGURE 12

$[Cu(DAPSC)(H_2O)_2]^{++}$ COMPLEX ION

The atomic numbering scheme and 50% probability thermal ellipsoids are shown. Primed atoms are related to unprimed atoms of the same designation by a two-fold axis passing through Cu, N1, and C3. Hydrogen atoms are omitted for clarity.

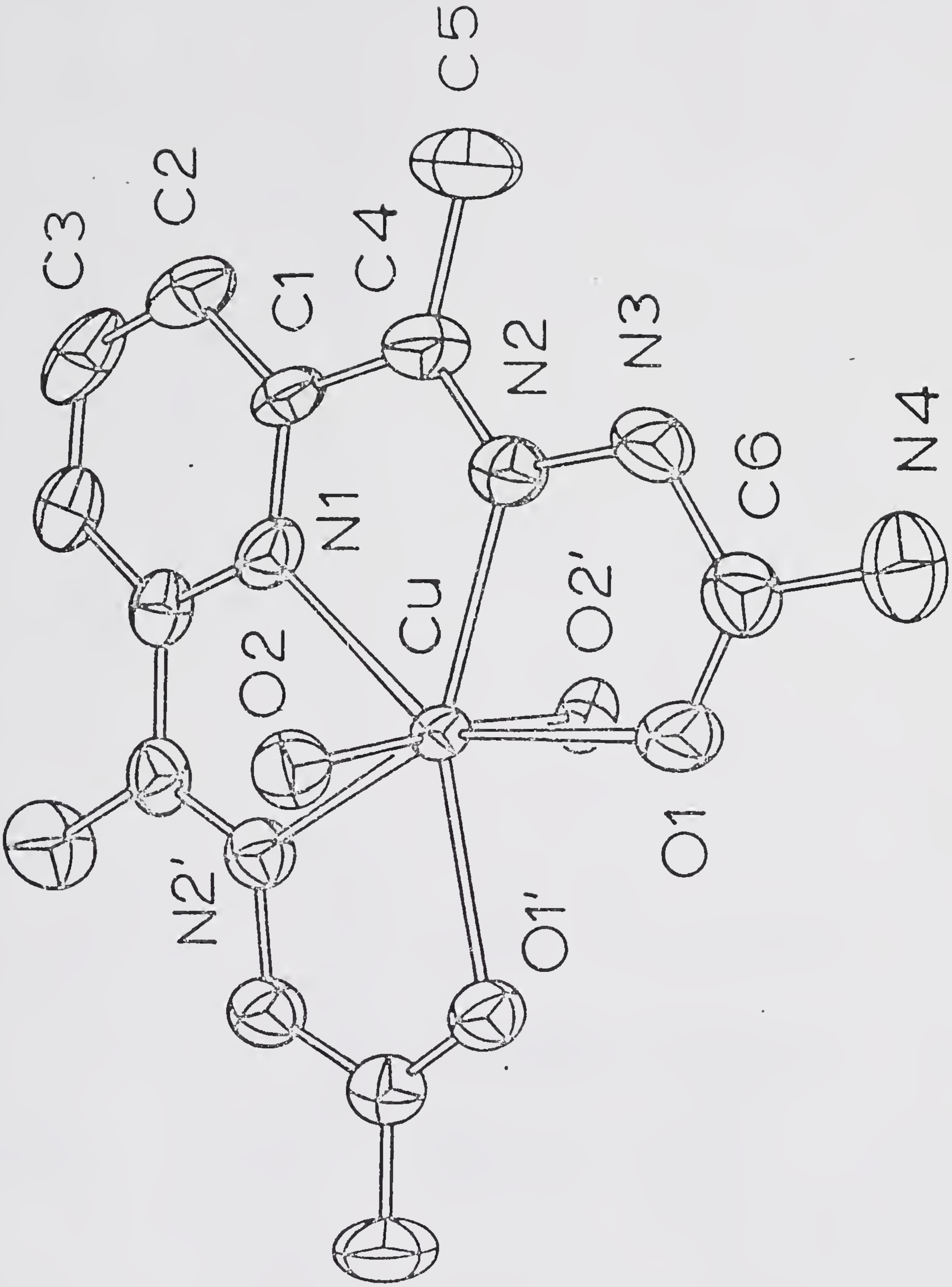

C5
C3
C2
C4
C1
N2
N3
N4
C6
N1
O2'
Cu
O2
O1
N2'
O1'

FIGURE 13

A PACKING DIAGRAM FOR $[Cu(DAPSC)(H_2O)_2](NO_3)_2 \cdot H_2O$

Dotted lines represent hydrogen bonds listed in Table 30. Hydrogen atoms and some atomic labels are omitted for clarity.

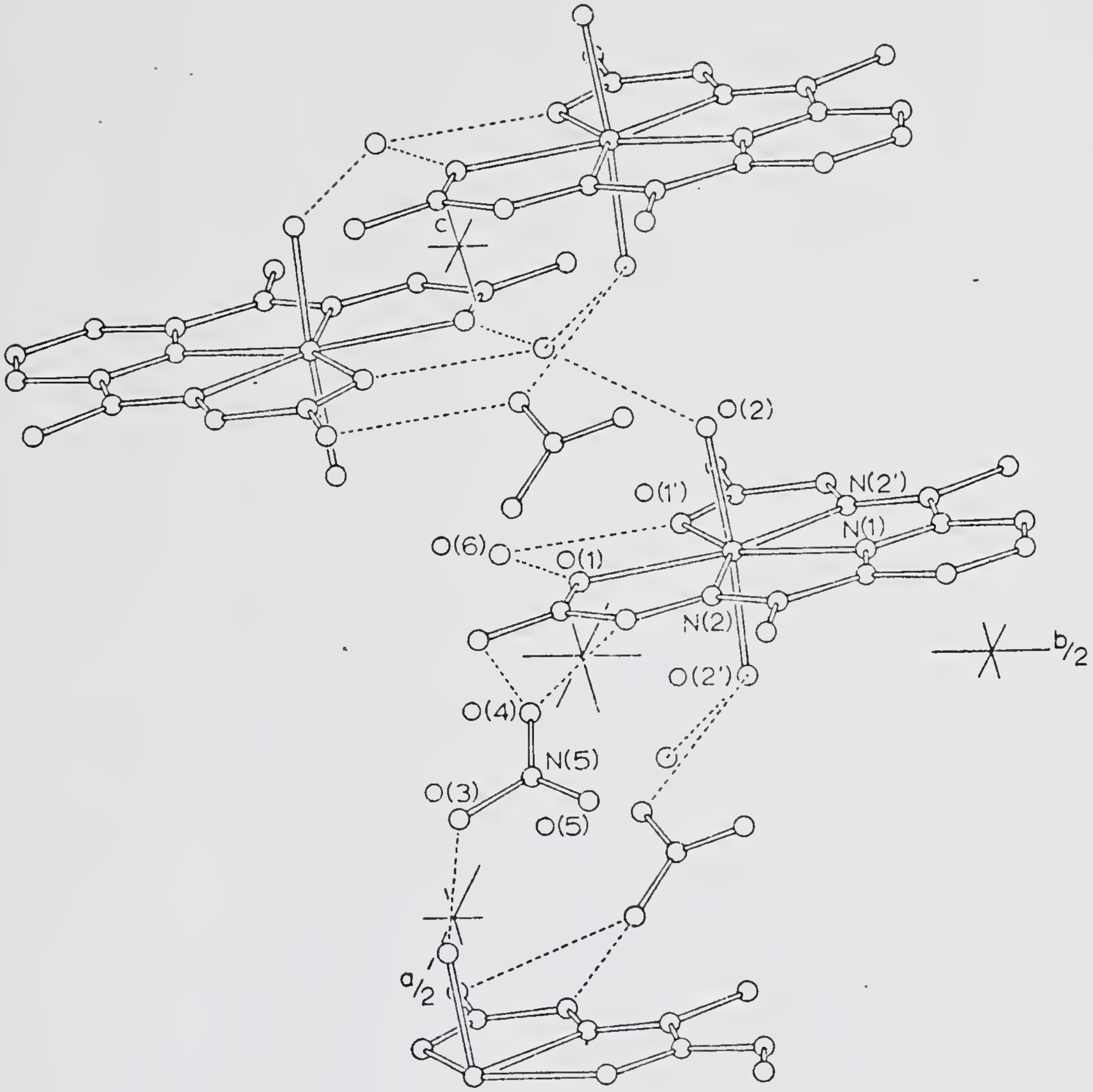

c
O(2)
O(1')
N(2')
N(1)
O(6)
O(1)
N(2)
O(2')
b/2
O(4)
N(5)
O(3)
O(5)
a/2

Table 33
METAL-LIGAND AND NON-BONDED CONTACT DISTANCES FOR SOME $[M(DAPSC)(H_2O)_2]^{++}$ COMPLEXES

The designations (e) and (a) refer to equatorial and axial donors respectively. Respective estimated standard deviations in parentheses follow the distances (Å).

	M=Mn	Ni	Cu
M-N (e)	2.30(1)	2.13(5)	2.26(1)
M-O (e)	2.21(1)	2.35(13)	2.35(1)
M-O (a)	2.23(4)	2.07(2)	1.92(1)
O(e)-O(a)	3.10(2)	3.01(5)	3.01(1)
N(e)-O(a)	3.23(2)	3.04(1)	3.01(3)
O(e)-O(e)	2.966(7)	2.805(8)	3.129(6)

scheme are shown in Figure 12. The ORTEP[58] packing diagram of the unit cell contents is illustrated in Figure 13.

Discussion

The pentagonal bipyramidal geometry of the complexes of DAPSC with Mn(II), Ni(II), and Cu(II) is easily seen in Figures 10 and 12. The atoms O1, O2, N1, N2, and N5 for Mn(II) and Ni(II) and atoms O1, O1', N1, N2, and N2' for Cu(II) form a planar pentagon around the central metal ion. The apical positions are occupied by water molecules in all cases.

The average metal-ligand bond distances in $[Mn(DAPSC)(H_2O)_2]^{++}$ do not differ significantly from those observed in $[Mn(DAPSC)(H_2O)Cl]^{+}$. Comparison of Table 33 with Table 10 and Figure 5 indicates that the non-bonded contacts for these species also are equivalent.

The metal-ligand bond distances in $[Ni(DAPSC)(H_2O)_2]^{++}$ are characterized as follows. The Ni-N1 bond distance of 2.060(6)Å is similar to other Ni-N(py) distances observed previously.[4,87,93-99] The Ni-N2 and Ni-N5 bond distances (2.222(6) and 2.108(6)Å, respectively) are somewhat longer than the distance usually found for Ni-N(imine) bonds.[4,87,96,97,99-101] The Ni-O(e) bonds (2.478(5)Å for O1 and 2.216(6)Å for O2) are much longer than similar bonds in other complexes of lower coordination number.[87,98,101-104] A suitable explanation for the large difference in the Ni-O(e) bond lengths has not been found. The Ni-O(a) bonds are within the range of Ni-OH_2 bonds for octahedral complexes.[87,93,94,98,102,104]

The metal-ligand bond distances in $[Cu(DAPSC)(H_2O)_2]^{++}$ fall into two categories. The Cu-DAPSC bonds are longer than previously observed bond lengths in complexes of lower coordination number for Cu-N(py)[105-110] (Cu-N1, 2.265(6)Å), Cu-N(imine)[80,105,111,112] (Cu-N2, 2.258(4)Å), and Cu-O(carboxyl)[73,113] bonds (Cu-O1, 2.350(4)Å). However, the copper-axial water bond of 1.922(3)Å is among the shortest reported for such a bond.[87]

The metal-ligand and non-bonded contact distances for the Mn(II), Ni(II), and Cu(II) complexes are compared in Table 33. The ionic radius of Mn(II) is apparently large enough that non-bonded contacts play a minor role in determining the bond distances. The contact distances for the Mn(II) complex are significantly longer than the sum of van der Waals radii for the atoms concerned. A familiar trend is displayed by the distances in the series Mn(II), Ni(II), Cu(II). The metal-nitrogen distances reach a minimum at Ni(II). This result is expected both on the basis of ionic radius and consideration of the orientation of the d orbitals into which electrons are added. Assuming all involved complexes are high spin, on going from Mn(II) to Co(II) the two additional electrons would be placed into the orbitals directed between the donors (d_{xz} and d_{yz}), according to the energy level diagram to be discussed later. In the Ni(II) complex an additional electron must be placed in an orbital directed at the planar donors (d_{xy} or $d_{x^2-y^2}$). In the Cu(II) complex the additional electron is added to an orbital directed at the planar donors and the metal-DAPSC distances increase relative to the Ni(II) complex as a result. The large estimated standard deviation of the Ni-O(e) bond renders a comparison of the M-O(e) meaningless. The trend of the axial ligand bond lengths is identical to that observed for the $[M(DAPSC)(H_2O)Cl]^+$ complexes. The distances decrease steadily from Mn(II) to Cu(II). The decrease on going from Mn(II) to Ni(II) may be explained by the decrease in ionic radius. However, the decrease observed going from Ni(II) to Cu(II) seems to be influenced by non-bonded contacts. While the non-bonded contacts remain relatively constant, the metal-DAPSC distances increase in the Cu(II) complex, allowing a closer approach of the axial ligands to the metal ion. The non-bonded contact between the equatorial oxygen atoms reaches a minimum in the Ni(II) complex, as expected.

Attention should be drawn to the small deviations from planarity as listed in Tables 26 and 31 for the DAPSC donor atoms in each of these complexes. As noted in Chapter 4, the complex $[Fe(DAPSC)Cl_2]Cl \cdot 2H_2O$ also contains a relatively planar DAPSC ligand when compared to the $[M(DAPSC)(H_2O)Cl]Cl \cdot 2H_2O$ complexes. The fact that each complex containing identical apical donors has a relatively planar DAPSC, while those complexes with two different apical donors have non-planar DAPSC ligands strongly suggests that the planarity of the DAPSC ligand is influenced by the nature of the apical donors.

For the Cu(II) complex, the arrangement of the donors about the copper atoms is staggered. Thus, N1 is on the plane, O1 and N2' are above the plane by 0.042Å and 0.031Å respectively, and the symmetry related atoms O1' and N2 are below the plane by the same values. The crystallographic symmetry of the complex cation imposes a helical array of donors with respect to the pyridine ring. For the Mn(II) and Ni(II) complexes the arrangement of donors is irregular. However, the deviations from planarity are approximately of the same order as the estimated standard deviations of the atomic coordinates and are not significant.

The packing diagrams for the structures appear in Figures 11 and 13. An outstanding feature of these diagrams is the extensive hydrogen bonding between the nitrate anions and the protons of both the ligand nitrogens and coordinated water molecules. Table 25 lists the ten hydrogen bonding interactions for the Mn(II) and Ni(II) structures. Four of these interactions involve nitrate-proton-amino nitrogen bonding. Three nitrate-proton-coordinated water interactions are present. For the Cu(II) structure, six hydrogen bonds are listed in Table 30. Three nitrate-proton-amino nitrogen and one nitrate-proton-coordinated water hydrogen bond are present. In all cases the distances are within the range expected.

CHAPTER 6
COMPLEXES FORMED WITH THE PENTADENTATE LIGANDS DAPPH AND DAPP

Heptacoordination for first-row transition metal ions cannot be considered commonplace. The possibility of producing PB complexes using the ligand DAPPH (Figure 1) appeared reasonable in view of the successful application of the planar DAPSC to producing this geometry. Deprotonation of DAPPH to produce the ligand DAPP was expected to result in a molecular complex containing a dinegative planar pentadentate ligand.[23,114] In this chapter, a pair of PB complexes with DAPPH as a planar pentadentate ligand are described. In addition, the structure of a deprotonated complex having twisted DAPP ligands, pyridine bridges, and a dimeric nature is also presented.

Solution and Refinement of Structure for $[M(DAPPH)(H_2O)_2]Cl_2$ (M=Co,Zn)

The cobalt atom was located in a sharpened three-dimensional Patterson function. A Fourier synthesis phased on the cobalt atom revealed the positions of two chlorine and two oxygen atoms. Subsequent Fourier syntheses established the approximate coordinates of the entire molecule. A difference Fourier synthesis at this point revealed no additional peaks, R=0.18. Three full matrix least-squares cycles using individual isotropic thermal parameters refined the structure, R=0.080. Three block diagonal least-squares cycles using individual anisotropic thermal parameters further reduced R to 0.060. All hydrogen atoms were found in a difference Fourier synthesis. These were arbitrarily assigned isotropic thermal parameters one unit larger than the atoms to which they were bonded. The structure was refined by three block diagonal least-squares cycles holding the hydrogen parameters constant, R=0.046. Less than 3% of the parameters had shifts of more than one-third of their respective estimated standard deviations and the refinement was terminated.

Similarity of the cell constants and scaled data suggested that the zinc and cobalt compounds were isomorphous. A difference Fourier synthesis calculated with the zinc data using the refined cobalt positional parameters revealed no significant discrepancies, R=0.18. Three full matrix least-squares cycles using the cobalt parameters as the initial coordinates and the isotropic thermal parameter estimated from the Wilson plot refined the structure, R=0.074. Three block diagonal least-squares cycles using individual anisotropic thermal parameters further reduced R to 0.056. A difference Fourier synthesis showed peaks corresponding to the hydrogen positions found in the isomorphous cobalt compound. Therefore, these coordinates and thermal parameters adjusted to the corresponding zinc parameters were assigned to the hydrogen atoms. Three least-squares cycles holding the hydrogen parameters constant reduced R to 0.040.

Since less than 3% of the parameters had shifts larger than their corresponding estimated standard deviations, refinement was terminated.

Results for [M(DAPPH)$(H_2O)_2$]Cl_2 (M=Co,Zn)

Final positional and thermal parameters for the non-hydrogen atoms of the two structures are given in Table 34. The probable positional parameters and carbon-hydrogen distances for the hydrogen atoms of [Co(DAPPH)$(H_2O)_2$]Cl_2 are tabulated in Table 35. Intramolecular bond distances and angles and short intermolecular distances appear in Table 36. Least-squares planes and deviations are in Table 37. The observed and calculated structure factors are listed in Table 38. Figure 14 is an ORTEP[58] diagram showing the complex ion and atomic numbering scheme. Figure 15 is an ORTEP[58] packing diagram of the unit cell.

Discussion

The DAPPH complexes of Co(II) and Zn(II) are isomorphous, differing only with respect to the central metal ion. The pentagonal bipyramidal arrangement of donors is easily seen in Figure 14. The atoms N1, N2, N4, N5, and N7 form a nearly planar pentagon, with atoms O1 and O2 occupying the apices. Figure 15 illustrates the hydrogen bonding and molecular packing of one half of the unit cell. The other half is related to the portion shown by a center of symmetry at (½,½,½).

Table 34
FINAL POSITIONAL AND THERMAL PARAMETERS (x 10^4) FOR THE NON-HYDROGEN ATOMS OF
$[M(DAPPH)(H_2O)_2]Cl_2$ (M = Co,Zn)
WITH THEIR RESPECTIVE ESTIMATED STANDARD DEVIATIONS IN PARENTHESES
The coordinates of the atoms for each structure are listed according
to the order of the metal atoms

ATOM	X	Y	Z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
M = Co	1352(1)	1331(1)	408(1)	94(1)	7(1)	42(1)	3(1)	27(1)	1(1)
Zn	1393(1)	1344(1)	348(1)	119(1)	10(1)	58(1)	2(1)	38(1)	2(1)
Cℓ1	6959(2)	669(1)	2113(1)	152(2)	11(1)	77(1)	20(1)	53(3)	9(1)
	7034(2)	698(1)	2056(1)	178(3)	12(1)	90(2)	18(1)	60(4)	11(1)
Cℓ2	5360(2)	1611(1)	7957(1)	145(2)	14(1)	75(1)	6(1)	79(3)	18(1)
	5418(2)	1610(1)	7917(1)	169(3)	16(1)	82(2)	0(1)	77(4)	19(1)
O1	4052(4)	1389(1)	488(3)	117(6)	14(1)	80(4)	13(3)	71(7)	15(2)
	4077(5)	1386(1)	410(4)	152(7)	16(1)	89(5)	10(4)	91(9)	25(3)
O2	-1353(4)	1324(1)	362(4)	116(6)	19(1)	86(4)	-8(3)	56(8)	8(3)
	-1289(5)	1349(2)	301(4)	134(7)	19(1)	96(5)	-13(4)	41(9)	16(3)
N1	2091(5)	1012(1)	2442(3)	100(6)	9(1)	46(4)	-2(3)	20(7)	2(2)
	2141(5)	1027(2)	2417(4)	119(8)	12(1)	55(4)	-1(4)	24(10)	6(3)
N2	1925(5)	529(1)	329(4)	114(7)	10(1)	51(4)	2(3)	7(8)	-2(2)
	1936(6)	526(2)	319(4)	143(9)	10(1)	62(5)	-2(4)	27(10)	-3(3)
N3	1794(6)	341(2)	-917(4)	189(9)	10(1)	57(4)	11(4)	20(9)	-6(3)
	1796(7)	327(2)	-902(5)	228(11)	13(1)	73(5)	9(5)	41(13)	-3(3)
N4	318(5)	1052(1)	-1719(4)	115(7)	9(1)	66(4)	3(3)	38(8)	-5(2)
	381(6)	1037(2)	-1780(4)	154(9)	10(1)	77(5)	2(4)	37(11)	-4(3)
N5	1310(5)	1906(1)	1943(4)	111(6)	9(1)	59(4)	2(3)	40(8)	1(2)
	1410(6)	1921(2)	1924(4)	130(8)	10(1)	70(5)	1(4)	51(10)	-1(3)

Table 34 - continued

ATOM	X	Y	Z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
N6	813(5)	2359(1)	1463(4)	174(8)	8(1)	58(4)	5(3)	66(9)	-2(2)
	939(6)	2369(2)	1451(4)	182(10)	11(1)	80(5)	6(4)	87(12)	-1(3)
N7	1256(5)	2079(1)	-529(4)	122(7)	8(1)	62(4)	7(3)	60(8)	-1(2)
	1309(6)	2095(2)	-576(4)	146(9)	10(1)	69(5)	4(4)	64(10)	-2(3)
C1	2683(6)	554(2)	2630(4)	101(7)	9(1)	53(4)	1(4)	16(9)	4(3)
	2722(7)	573(2)	2610(5)	114(10)	12(1)	74(6)	-3(5)	18(12)	16(4)
C2	3303(7)	358(2)	3915(5)	159(10)	11(1)	68(5)	7(4)	38(11)	8(3)
	3337(8)	383(2)	3890(6)	188(13)	15(1)	74(6)	1(6)	14(15)	10(4)
C3	3281(7)	644(2)	5008(5)	170(10)	16(1)	59(5)	19(5)	36(12)	18(4)
	3345(9)	671(3)	4972(6)	211(14)	18(1)	76(7)	16(6)	45(16)	14(4)
C4	2657(7)	1116(2)	4808(5)	141(9)	14(1)	54(5)	1(4)	40(11)	4(3)
	2714(8)	1134(2)	4775(6)	165(11)	17(1)	63(6)	-2(6)	50(13)	1(4)
C5	2068(6)	1290(2)	3513(4)	91(7)	11(1)	52(4)	-6(4)	41(9)	-2(3)
	2137(7)	1311(2)	3468(5)	118(10)	12(1)	55(5)	-3(5)	28(11)	1(3)
C6	2612(6)	282(2)	1376(4)	110(8)	8(1)	59(5)	-6(3)	8(9)	7(3)
	2630(7)	294(2)	1379(5)	137(11)	12(1)	73(6)	-2(5)	15(13)	3(4)
C7	3323(7)	-223(2)	1412(5)	187(11)	9(1)	79(5)	3(4)	26(12)	4(3)
	3375(9)	-204(2)	1448(6)	222(14)	11(1)	109(7)	-1(6)	60(17)	6(4)
C8	806(6)	602(2)	-1975(5)	115(8)	7(1)	65(5)	6(3)	42(10)	-4(3)
	809(7)	588(2)	-1984(5)	138(10)	11(1)	70(6)	3(5)	43(13)	-9(3)
C9	311(7)	382(2)	-3230(5)	158(9)	12(1)	62(5)	17(5)	44(11)	-10(3)
	331(8)	348(2)	-3209(6)	215(14)	12(1)	89(7)	14(6)	62(16)	-6(4)

Table 34 - continued

ATOM	X	Y	Z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
C10	-768(8)	631(2)	-4263(5)	198(11)	14(1)	60(5)	18(5)	40(12)	-4(3)
	-736(9)	602(2)	-4275(6)	247(15)	17(1)	74(7)	6(7)	39(16)	-3(4)
C11	-1339(7)	1090(2)	-4010(5)	151(10)	15(1)	68(5)	18(5)	16(11)	4(4)
	-1267(8)	1062(2)	-4074(6)	183(12)	15(1)	81(7)	17(6)	14(14)	7(4)
C12	-786(6)	1285(2)	-2743(5)	131(8)	9(1)	81(5)	14(4)	48(11)	0(3)
	-715(8)	1262(2)	-2831(6)	171(12)	11(1)	91(7)	1(5)	56(15)	-3(4)
C13	1481(6)	1796(2)	3190(4)	108(8)	10(1)	60(5)	1(4)	52(10)	-4(3)
	1559(7)	1812(2)	3156(5)	122(10)	13(1)	71(6)	-6(5)	65(12)	-8(4)
C14	1153(8)	2130(2)	4234(5)	241(13)	13(1)	68(5)	19(5)	105(14)	-9(3)
	1214(9)	2135(2)	4193(6)	221(14)	16(1)	91(7)	10(6)	97(16)	-9(4)
C15	927(6)	2452(2)	174(4)	108(8)	9(1)	50(4)	5(3)	32(9)	-3(3)
	1038(6)	2465(2)	163(5)	111(9)	10(1)	63(6)	7(4)	31(12)	1(3)
C16	712(7)	2932(2)	-288(5)	145(9)	8(1)	77(5)	3(4)	52(11)	0(3)
	867(7)	2940(2)	-294(6)	152(11)	10(1)	87(6)	-2(5)	56(13)	-1(4)
C17	898(7)	3028(2)	-1544(5)	190(11)	10(1)	76(5)	3(5)	68(12)	9(3)
	1012(8)	3034(2)	-1564(6)	196(13)	12(1)	94(7)	8(6)	63(15)	11(4)
C18	1334(7)	2647(2)	-2282(5)	193(11)	12(1)	66(5)	-1(5)	88(12)	0(3)
	1361(9)	2658(2)	-2328(6)	230(14)	14(1)	71(6)	3(6)	112(15)	5(4)
C19	1513(6)	2187(2)	-1747(5)	151(9)	9(1)	60(5)	0(4)	60(11)	0(3)
	1516(8)	2202(2)	-1793(5)	177(12)	11(1)	74(6)	-4(5)	85(14)	-5(4)

Table 35

POSITIONAL AND THERMAL PARAMETERS (x 10^3) FOR THE HYDROGEN ATOMS OF $[Co(DAPPH)(H_2O)_2]Cl_2$

ATOM	BONDED TO	DISTANCE, Å	X	Y	Z	B(Å^2)
H1	C2	1.02	368	0	400	4.4
H2	C3	1.10	373	50	604	4.9
H3	C4	1.00	279	132	563	4.2
H4	C7	0.99	280	-42	200	4.4
H5	C7	0.88	283	-39	68	4.4
H6	C7	1.02	461	-16	153	4.4
H7	C14	1.08	11	230	347	4.9
H8	C14	0.81	157	240	439	4.9
H9	C14	0.93	32	199	459	4.9
H10	N3	1.05	215	0	-126	4.4
H11	C9	1.09	88	2	-334	4.3
H12	C10	1.04	-136	48	-520	4.8
H13	C11	0.97	-219	130	-462	4.7
H14	C12	0.96	-118	160	-250	4.1
H15	N6	0.99	64	264	203	4.0
H16	C16	0.98	64	319	36	4.1
H17	C17	1.04	90	337	-198	4.4
H18	C18	1.00	137	269	-324	4.5
H19	C19	1.09	192	188	-227	3.8
H20	O1	0.84	436	149	-19	4.2
H21	O1	0.97	481	113	94	4.2
H22	O2	0.81	-217	136	-29	4.8
H23	O2	0.86	-179	115	89	4.8

Table 36

INTRAMOLECULAR BOND DISTANCES AND ANGLES AND SHORT INTERMOLECULAR CONTACTS FOR $[M(DAPPH)(H_2O)_2]Cl_2$ (M=Co,Zn) WITH THEIR ESTIMATED STANDARD DEVIATIONS IN PARENTHESES

(a) Bond Distances (Å)

	M=Co	Zn		M=Co	Zn
M-O1	2.146(4)	2.104(4)	N7-C15	1.320(6)	1.332(7)
M-O2	2.153(4)	2.103(4)	N7-C19	1.361(6)	1.348(7)
M-N1	2.207(4)	2.251(4)	C1-C2	1.396(7)	1.393(8)
M-N2	2.248(4)	2.314(4)	C1-C6	1.484(6)	1.478(8)
M-N4	2.268(4)	2.305(4)	C2-C3	1.378(8)	1.376(9)
M-N5	2.242(4)	2.286(4)	C3-C4	1.382(8)	1.375(10)
M-N7	2.258(4)	2.288(4)	C4-C5	1.381(6)	1.401(8)
N1-C1	1.335(6)	1.338(7)	C5-C13	1.473(7)	1.472(8)
N1-C5	1.349(6)	1.346(7)	C6-C7	1.492(7)	1.496(8)
N2-N3	1.365(5)	1.359(6)	C8-C9	1.390(7)	1.395(8)
N2-C6	1.271(6)	1.267(7)	C9-C10	1.366(8)	1.393(9)
N3-C8	1.368(6)	1.391(7)	C10-C11	1.385(8)	1.375(10)
N4-C8	1.340(6)	1.321(7)	C11-C12	1.375(7)	1.366(8)
N4-C12	1.345(6)	1.353(7)	C13-C14	1.490(7)	1.482(8)
N5-N6	1.356(6)	1.352(6)	C15-C16	1.394(7)	1.395(8)
N5-C13	1.296(6)	1.289(7)	C16-C17	1.372(7)	1.377(8)
N6-C15	1.384(6)	1.385(7)	C17-C18	1.390(8)	1.381(9)
			C18-C19	1.368(7)	1.376(8)

(b) Bond Angles (°)

	M=Co	Zn		M=Co	Zn
O1-M-O2	176.1(1)	176.5(2)	N5-N6-C15	115.6(4)	116.5(4)
O1-M-N1	88.9(1)	89.0(2)	M-N7-C15	117.0(3)	116.9(3)
O1-M-N2	82.0(1)	82.3(2)	M-N7-C19	126.7(3)	126.5(4)
O1-M-N4	99.6(1)	98.1(2)	C15-N7-C19	116.3(4)	116.6(5)
O1-M-N5	97.2(1)	97.1(2)	N1-C1-C2	121.5(4)	121.2(5)
O1-M-N7	82.4(1)	83.2(2)	N1-C1-C6	114.4(4)	115.2(5)
O2-M-N1	91.8(1)	92.0(2)	C2-C1-C6	124.1(4)	123.6(5)
O2-M-N2	101.8(1)	101.2(2)	C1-C2-C3	119.0(5)	119.0(6)

Table 36 - continued

(b) continued

	M=Co	Zn		M=Co	Zn
O2-M-N4	82.5(1)	83.5(2)	C2-C3-C4	119.4(5)	119.8(6)
O2-M-N5	79.5(1)	80.2(2)	C3-C4-C5	118.9(5)	119.0(6)
O2-M-N7	94.5(1)	93.8(2)	N1-C5-C4	121.8(4)	120.7(5)
N1-M-N2	69.1(1)	68.0(2)	N1-C5-C13	114.7(4)	116.2(5)
N1-M-N4	136.7(1)	135.0(2)	C4-C5-C13	123.4(4)	123.1(5)
N1-M-N5	69.8(1)	69.0(2)	N2-C6-C1	112.6(4)	113.4(5)
N1-M-N7	137.5(1)	136.7(2)	N2-C6-C7	126.2(4)	125.7(5)
N2-M-N4	70.2(1)	69.1(2)	C1-C6-C7	121.2(4)	120.8(5)
N2-M-N5	138.9(1)	127.0(2)	N3-C8-N4	117.4(4)	118.3(5)
N2-M-N7	148.6(1)	150.9(2)	N3-C8-C9	118.8(4)	116.5(5)
N4-M-N5	148.5(1)	151.6(2)	N4-C8-C9	123.8(4)	125.2(5)
N4-M-N7	85.8(1)	88.3(2)	C8-C9-C10	118.5(5)	116.4(6)
N5-M-N7	70.2(1)	69.9(2)	C9-C10-C11	118.6(5)	119.5(6)
M-N1-C1	120.4(3)	120.3(4)	C10-C11-C12	119.5(5)	119.0(6)
M-N1-C5	120.0(3)	119.2(3)	N4-C12-C11	123.0(5)	123.5(6)
C1-N1-C5	119.4(4)	120.2(5)	N5-C13-C5	112.8(4)	112.6(5)
M-N2-N3	115.9(3)	116.1(3)	N5-C13-C14	125.9(4)	126.2(5)
M-N2-C6	122.32(3)	121.7(4)	C5-C13-C14	121.3(4)	121.2(5)
N3-N2-C6	120.7(4)	121.0(5)	N6-C15-N7	117.5(4)	117.8(5)
N2-N3-C8	116.2(4)	115.6(5)	N6-C15-C16	118.0(4)	119.0(5)
M-N4-C8	116.7(3)	117.7(4)	N7-C15-C16	124.5(4)	123.2(5)
M-N4-C12	126.8(3)	126.1(4)	C15-C16-C17	118.0(5)	118.6(5)
C8-N4-C12	116.5(4)	116.1(5)	C16-C17-C18	118.8(5)	119.1(6)
M-N5-N6	116.2(3)	115.8(3)	C17-C18-C19	118.9(5)	118.2(6)
M-N5-C13	121.6(3)	121.7(4)	N7-C19-C18	123.3(5)	124.1(5)
N6-N5-C13	121.3(4)	121.5(5)			

(c) Short Intermolecular Contacts (Å)

ATOM A	EQUIV.POS.	ATOM B	EQUIV.POS.	DIST(M=Co)	(M=Zn)
Cℓ1	X,Y,Z	O1	X,Y,Z	3.170(4)	3.148(4)
O2	1+X,Y,Z	Cℓ1	X,Y,Z	3.102(4)	3.097(4)
O1	X,Y,Z	Cℓ2	X,Y,Z-1	3.127(4)	3.104(4)
O2	1+X,Y,Z	Cℓ2	X,Y,Z-1	3.202(4)	3.165(4)

Table 36 - continued

BOND	ANGLE	
	Co	Zn
O1-H20-Cℓ2	168.1(2)°	164.9(3)°
O1-H21-Cℓ1	167.0(2)	163.4(2)
O2-H22-Cℓ2	169.1(3)	164.6(3)
O2-H23-Cℓ1	174.9(3)	176.0(2)

Table 37
LEAST-SQUARES PLANES AND DEVIATIONS FOR $[M(DAPPH)(H_2O)_2]Cl_2$ (M=Co,Zn)

The titles of the planes are given, followed by the dihedral angles (°) between the planes. The deviations (x 10^3 Å) of selected atoms from the planes are given. Asterisks denote deviations of atoms used to define the plane. The equations of the planes are of the form ax+by+cz=d, where d is the distance (Å) from the origin.

Plane 1. Plane Through Pentagonal Donor Set.

Plane 2. Plane Through Pyridine Ring of DAP Residue.

Plane 3. Plane Through Pyridine Ring Containing C8-C12.

Plane 4. Plane Through Pyridine Ring Containing C15-C19.

Dihedral Angles Between Planes

PLANE A	PLANE B	ANGLE	
		M=Co	Zn
1	2	13.61	13.65
1	3	24.22	22.73
1	4	23.13	21.03
2	3	16.91	16.05
2	4	23.50	22.52
3	4	40.40	38.32

Table 37 - continued

	PLANE 1		PLANE 2		PLANE 3	
	M=Co	Zn	M=Co	Zn	M=Co	Zn
a	0.9949	0.9964	0.9434	0.9486	0.8820	0.9014
b	0.0987	0.0823	0.3295	0.3149	0.4051	0.3601
c	0.0230	0.0225	0.0370	0.0310	-0.2406	-0.4066
d	1.3310	1.3148	1.9462	1.9480	2.2011	2.1460
M	3	0	185	189	32	13
N1	-3*	0*	4*	2*	-779	-773
N2	262*	247*	-89	-113	-414	-400
N4	-364*	-335*	-375	-352	19*	27*
N5	-259*	-247*	331	348	-99	-159
N7	363*	335*	995	494	1246	1159

ATOM	DEV.	ATOM	DEV.	ATOM	DEV.	ATOM	DEV.	ATOM	DEV.	ATOM	DEV.
O1	2148	O1	2103	C1	-4*	C1	-5*	C8	-13*	C8	-18*
O2	-2141	O2	-2095	C2	2*	C2	-1*	C9	-2*	C9	-2*
				C3	0*	C3	10*	C10	11*	C10	12*
				C4	-1*	C4	-13*	C11	-5*	C11	-3*
				C5	-1*	C5	7*	C12	10*	C12	-16*

Table 37 - continued - extended

PLANE 4

M=Co		Zn	
0.8987		0.9173	
0.1645		0.1331	
0.4066		0.3752	
1.7818		1.6701	
-145		-122	
566		562	
-107		-35	
-1352		-1235	
327		302	
-26*		-22*	
ATOM	DEV.	ATOM	DEV.
C15	17*	C15	12*
C16	5*	C16	6*
C17	-17*	C17	-14*
C18	8*	C18	4*
C19	14*	C19	14*

Table 38

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $[M(DAPPH)(H_2O)_2]Cl_2$ (M=Co,Zn)

The structure factors for the reflection (HKL) are listed to the right of the appropriate L value under the corresponding H and K values. FO and FC refer to F_{obs} and F_{calc} respectively. The structure factors for the Co compound are listed first.

```
   L    FO      FC

H=     0,  K=     0

   2   103      93
   4  1141    1059
   6   329     317
   8   510    -492
  10   149    -170

H=     1,  K=     0

   1   237     236
   3   -48      -1
   5   248    -279
   7   126     127
   9   727    -729
  11   155    -155
 -11   184    -186
  -9   235     243
  -7   715     712
  -5   667     663
  -3  1744    1812
  -1  1762    1887

H=     2,  K=     0

   0   599    -587
   2   431     421
   4   424    -433
   6   119    -112
   8   614    -604
  10   225    -187
 -12   -66      93
 -10   500     489
  -8   -56     -24
  -6   554     579
  -4   -47     -29
  -2  1092   -1092

H=     3,  K=     0

   1  1301   -1368
   3   954    -948
   5   653    -664
   7   -56       7
   9   283     276
 -11   341     353
  -9   156    -121
  -7   432     423
  -5    70      73
  -3   520    -511
  -1  1049   -1057

H=     4,  K=     0

   0  1219   -1186
   2   678    -696
   4   267    -265
   6   645     655
   8   105      80
 -12   174     174
 -10    88      67
  -8   641     635
  -6   877    -868
  -4   115    -101
  -2  1462   -1472

H=     5,  K=     0

   1   377    -399
   3   638     664
   5   304    -297
   7   278     290
 -11   179     190
  -9   -57     -72
  -7   304    -312
  -5   582    -596
  -3   115     -96
  -1   118    -110
```

```
   L    FO      FC

H=     6,  K=     0

   0   128     149
   2   154     157
   4    81      71
   6   133     128
 -10   -62      50
  -8   395    -393
  -6   130    -126
  -4   -52     -63
  -2   163    -154

H=     7,  K=     0

   1   433     427
   3   224     202
   5   169     169
  -9   243    -231
  -7   321    -333
  -5   -56      28
  -3   -54      41
  -1   289     272

H=     8,  K=     0

   0   110     118
   2   265     260
  -8   -62      47
  -6   -60     -73
  -4   386     383
  -2   316     316

H=     9,  K=     0

  -7   -64      72
  -5   260     260
  -3   -61      -5
  -1   181     178

H=     0,  K=     1

   1  1107    1065
   2   171     181
   3   199    -199
   4  1017    -990
   5   659     659
   6   374    -343
   7   477    -443
   8   323    -316
   9   160    -164
  10   257    -263
  11   341    -330

H=     1,  K=     1

   0   889     913
   1   909    -912
   2   666     625
   3   402    -400
   4   383    -367
   5   248    -244
   6   -51     -62
   7   246    -246
   8   744    -725
   9   158     152
  10   233    -237
  11   -63      14
 -12   -66     -12
 -11   371     359
 -10   124    -113
  -9   303     305
  -8   356     345
  -7   394     389
  -6    86      93
  -5   -50     105
  -4   449     452
  -3   149    -163
  -2   -49      48
  -1   626    -624
```

```
   L    FO      FC

H=     2,  K=     1

   0  2241   -2341
   1   402    -411
   2   366     355
   3   114     111
   4   505    -513
   5   366    -421
   6   -51      14
   7   136    -124
   8   157     185
   9   125    -125
  10   196     192
 -12   112     135
 -11   170     148
 -10   125     128
  -9   179     195
  -8   545     541
  -7   383     385
  -6   791    -786
  -5   678     667
  -4   -47      15
  -3   -48      41
  -2   144     125
  -1    75     -28

H=     3,  K=     1

   0   398    -409
   1  1117   -1137
   2   731    -748
   3   289     299
   4   197    -184
   5   -51      -8
   6   171    -173
   7   253     252
   8    97      71
   9   312     328
  10   -65      54
 -12   138     142
 -11   267     275
 -10   366     371
  -9   149    -149
  -8   295     293
  -7   481    -493
  -6   577     562
  -5  1712    -532
  -4   295    -309
  -3   709    -760
  -2   580    -574
  -1   921    -939

H=     4,  K=     1

   0   -48     -53
   1    88      50
   2   257     257
   3   836    -837
   4   323     322
   5   -54      12
   6   202     203
   7   286     293
   8   152     148
   9   138     149
 -12   -69    -114
 -11   -64      61
 -10   382    -395
  -9   364     359
  -8   345    -352
  -7   408    -402
  -6   799    -802
  -5   371    -371
  -4   221    -215
  -3   144    -137
  -2   398    -413
  -1   947    -938

H=     5,  K=     1

   0   430    -439
```

```
   L    FO      FC

   1   227     215
   2    93      74
   3   191     166
   4   -56      30
   5   192     188
   6   203     220
   7   -60     -69
   8   214     223
 -11   235    -229
 -10   240    -253
  -9   -59     -64
  -8   167    -168
  -7   416    -423
  -6   205    -206
  -5   236     242
  -4   489    -499
  -3   -43     -53
  -2   210     220
  -1   337     345

H=     6,  K=     1

   0    83      93
   1   252     256
   2   374     403
   3   222     222
   4   -57     -43
   5    92     103
   6   -52     -76
   7   -64      24
 -11   193    -156
 -10   151    -134
  -9   -58       8
  -8   -59     -38
  -7   358    -354
  -6   -56      74
  -5    82     103
  -4   245     256
  -3   143    -140
  -2   361     356
  -1   -52      49

H=     7,  K=     1

   0   294     314
   1   115     110
   2   244     252
   3   164    -153
   4   133     143
   5   111     -71
 -10   -63     -76
  -9    93      74
  -8   162    -180
  -7   158     164
  -6   -55      73
  -5   545     559
  -4   118     117
  -3   -54      48
  -2   -55      95
  -1   323     337

H=     8,  K=     1

   0   171    -177
   1   257     255
   2   -61     -44
   3   -64      52
  -9   110     -77
  -8   377     379
  -7   150     153
  -6    97     105
  -5   -57      54
  -4   -58      44
  -3   301     308
  -2   117     142
  -1   -58      -7

H=     9,  K=     1

   0   -61      35
```

```
    L    FO     FC

   -7   -65     28
   -6   199    197
   -5   -61     50
   -4    95    -69
   -3   -60    -29
   -2   154    160
   -1   -61    -63

 H=     0,  K=     2

    0    88     49
    1   527   -503
    2   199   -193
    3   766   -762
    4   294   -280
    5  1088  -1052
    6   303   -274
    7   671   -640
    8   230    235
    9   675   -687
   10   128    129
   11   -63    -77

 H=     1,  K=     2

    0  1480  -1479
    1   603   -584
    2  1403  -1351
    3    88    -85
    4   591   -548
    5   215   -180
    6   718   -684
    7   -53    -36
    8   -57    -65
    9   167   -168
   10   -62     94
   11   169    190
  -12   -67     79
  -11   -64    -10
  -10   631    625
   -9   453    438
   -8   160    158
   -7   255   -311
   -6   426    430
   -5   199   -197
   -4    78    -73
   -3   390    377
   -2   362   -364
   -1   495   -466

 H=     2,  K=     2

    0  1302  -1347
    1   423    398
    2   141   -124
    3   613   -612
    4    75    -84
    5   190   -196
    6   241   -250
    7   529    530
    8   106    -85
    9   -58    -17
   10   -64    -36
  -12   -66     75
  -11   -62     60
  -10   -58    -30
   -9   -59     -4
   -8   274   -284
   -7   205    223
   -6   437    442
   -5   706   -721
   -4   269   -279
   -3   736    736
   -2   267    252
   -1  2435  -2592

 H=     3,  K=     2

    0    94     42
    1   316    328
```

```
    L    FO     FC

    2   260   -277
    3   407   -406
    4   778    784
    5   235    241
    6   -55     91
    7   -58    -60
    8   609    605
    9   -60     65
   10   159    202
  -12   -68    100
  -11   192   -196
  -10   -60    -50
   -9   -58    -52
   -8   173   -159
   -7   329   -325
   -6   324   -323
   -5   589    584
   -4   938   -968
   -3   370   -364
   -2   592   -620
   -1   499   -515

 H=     4,  K=     2

    0   782    794
    1   635    658
    2   -48     -5
    3   770    756
    4   -53     13
    5   365    381
    6   208    215
    7   518    512
    8   -62    -76
    9   115    104
  -12   -65     26
  -11   250   -247
  -10   233   -248
   -9   -59    -91
   -8   -57    -48
   -7   785   -806
   -6   -53    -73
   -5   470   -491
   -4   285    293
   -3   -48     56
   -2   195   -194
   -1   105    120

 H=     5,  K=     2

    0   532    537
    1   434    436
    2   456    456
    3   144    129
    4   203    207
    5    86    -94
    6    94    101
    7   123    118
    8   123   -141
  -11    90    -51
  -10   157   -122
   -9   -58     12
   -8   421   -425
   -7   -57     83
   -6    91    -94
   -5   119    125
   -4   336    357
   -3   290    284
   -2    70    -37
   -1   210    212

 H=     6,  K=     2

    0   192    183
    1   130    142
    2   144    127
    3   292    299
    4   113    112
    5   294   -304
    6   101   -117
    7   -64     30
```

```
    L    FO     FC

  -11   -66    -72
  -10   137    136
   -9   322   -319
   -8   -58     51
   -7   297    302
   -6   292    302
   -5   122   -118
   -4   221   -235
   -3   364    378
   -2   235    234
   -1   252    268

 H=     7,  K=     2

    0   258    257
    1   166    167
    2   239   -239
    3   130   -125
    4   -60    -28
    5   -64    -23
  -10   179    184
   -9   143    135
   -8   -61     20
   -7    96     80
   -6   267    263
   -5   -58    -44
   -4   467    470
   -3   100    107
   -2   204    203
   -1   181   -158

 H=     8,  K=     2

    0   185   -196
    1   236   -234
    2   -62    -52
    3   132   -130
   -9   218    214
   -8   125    117
   -7   265    265
   -6   126     77
   -5   161    187
   -4   184   -177
   -3   166    167
   -2    85     81
   -1   123   -143

 H=     9,  K=     2

    0   189   -179
   -6   -62    -24
   -5   -61    -19
   -4    89    -66
   -3   -58    -13
   -2   147   -125
   -1   -62    -11

 H=     0,  K=     3

    1   810   -773
    2   825   -800
    3   607   -633
    4   809   -785
    5   583   -579
    6   969   -965
    7   425    424
    8   -56    -56
    9   265    256
   10   123   -142
   11   161    161

 H=     1,  K=     3

    0   437   -419
    1   820    813
    2   452   -444
    3   625   -612
    4   263    256
    5   152    172
    6   513    483
```

```
    L    FO     FC

    7    83    -80
    8   122   -120
    9   -56    -25
   10   321    328
   11   -63     26
  -12   -64      3
  -11    93     48
  -10   113    133
   -9   617    602
   -8    33     75
   -7   261    259
   -6   448   -460
   -5  1036   1035
   -4   278   -240
   -3   545   -513
   -2   523   -585
   -1   619   -615

 H=     2,  K=     3

    0   759    745
    1   292    302
    2   534    504
    3   940    940
    4   543   -533
    5   160   -162
    6   260    246
    7   218    226
    8   110    108
    9   177    164
   10   167    156
  -12   244    229
  -11   -61    -38
  -10   -58     -2
   -9   238   -248
   -8   208    198
   -7   -53    -38
   -6   298   -299
   -5   281   -301
   -4   283    268
   -3   255    246
   -2   271    268
   -1  1384  -1372

 H=     3,  K=     3

    0  1772   1773
    1   103    -98
    2   390    385
    3   252    245
    4   329    334
    5    96    104
    6   401    414
    7   627    629
    8   -60      7
    9   268    268
   10   -63     50
  -12   262   -273
  -11   169    172
  -10   190   -215
   -9   371   -391
   -8   622   -620
   -7   -55    -76
   -6   146   -177
   -5   305   -311
   -4   269    252
   -3   317   -333
   -2   570   -567
   -1   340   -370

 H=     4,  K=     3

    0   633    652
    1   441    439
    2   396    374
    3   436    431
    4   571    576
    5   -54    -16
    6   192    211
    7   -59     59
   L    FO     FC

   8   179    158
   9   164   -159
 -12   -67    -79
 -11   265   -258
 -10   210   -209
  -9   364   -379
  -8   234   -224
  -7   -56     70
  -6   667   -678
  -5   -50     57
  -4   326   -341
  -3   968    975
  -2   390   -390
  -1  1101   1115

H=     5,  K=    3

   0   153    132
   1   261    281
   2   147    151
   3   185    207
   4   127   -150
   5   -57     48
   6   -59    -79
   7   -62     69
   8   255   -250
 -11   218   -215
 -10   145    150
  -9   -59    -34
  -8   -58     61
  -7    84    -87
  -6   -53    -46
  -5   147   -139
  -4   530    533
  -3   395    400
  -2   231    244
  -1   102    118

H=     6,  K=    3

   0   374   -388
   1   392   -403
   2   287    301
   3   -54    -23
   4   -57     60
   5   269   -274
   6   146   -166
   7   228   -229
 -11   267    268
 -10   -62    -16
  -9   115   -107
  -8   159    159
  -7   291    290
  -6   234    257
  -5   131    103
  -4   115    -95
  -3    86    -77
  -2   478    497
  -1   109    121

H=     7,  K=    3

   0   419   -442
   1   119   -141
   2   312   -326
   3   130   -117
   4   153   -173
   5   161   -161
 -10   -63     65
  -9   -65    121
  -8   538    530
  -7   136    118
  -6   132   -122
  -5   328    325
  -4   -57    -23
  -3   -55    -23
  -2   421   -426
  -1   255    252

H=     8,  K=    3
```

```
   L    FO     FC


   0   110    -97
   1   329   -332
   2   202   -227
   3    93     33
  -9   -65     61
  -8   201    183
  -7   -62     13
  -6    92    -63
  -5   241   -247
  -4   196    188
  -3   361   -373
  -2   -57    -35
  -1   159   -148

H=     9,  K=    3

   0   106    -91
  -6   138   -145
  -5   -60    -29
  -4   -62    -87
  -3   -62     17
  -2   -61     -2
  -1   -64    -96

H=     0,  K=    4

   0  1207  -1128
   1   129   -107
   2   659   -629
   3  1102   1059
   4  1118  -1108
   5   402   -390
   6   101     96
   7   234    244
   8   333    315
   9   -57    -39
  10   229    222
  11   175   -181

H=     1,  K=    4

   0   -47     68
   1   612    578
   2   115   -132
   3   356   -338
   4   777   -759
   5   749    718
   6   360    354
   7   220    207
   8   447   -459
   9   452    446
  10   181    184
  11   -63     97
 -12   167   -167
 -11   -63     66
 -10   141   -135
  -9   173    167
  -8   299   -315
  -7   494   -473
  -6   354   -355
  -5   685   -672
  -4   644    647
  -3   656   -662
  -2   588   -536
  -1   629   -611

H=     2,  K=    4

   0   -49    -42
   1   -49    -39
   2   386    374
   3    77    -33
   4   723    694
   5   175    162
   6   428    439
   7    84    100
   8   320    328
   9   -58    -27
  10   -62    -28
```

```
   L    FO     FC

 -12   135    104
 -11   -63    -19
 -10   251   -228
  -9   342   -353
  -8   140   -125
  -7   -53      8
  -6   308   -298
  -5   162   -155
  -4   364   -357
  -3   127    129
  -2   439    441
  -1  1551  -1575

H=     3,  K=    4

   0   153    132
   1   732    751
   2   696    705
   3   682    704
   4   -49    -10
   5   620    612
   6   266   -265
   7   100     85
   8   158    159
   9   118   -104
  10   157   -184
 -12   106     62
 -11   395   -401
 -10   172   -157
  -9   138   -127
  -8   -57    -28
  -7   366   -376
  -6   217   -203
  -5   232   -238
  -4    69   -116
  -3   636    650
  -2   456    471
  -1   115    113

H=     4,  K=    4

   0   250    249
   1   416   -395
   2   332    324
   3   114   -132
   4   272    264
   5   121    105
   6   321   -308
   7   208   -201
   8   150   -143
   9   196    186
 -12   281   -278
 -11   -66     87
 -10   211   -206
  -9   205    283
  -8   154   -167
  -7    83   -109
  -6   283    289
  -5   592    591
  -4   -48     47
  -3   418   -427
  -2  1218   1233
  -1   868    884

H=     5,  K=    4

   0   698   -697
   1   -50    -37
   2   383    366
   3   220   -218
   4   140   -140
   5   192   -188
   6    91    -59
   7   242   -244
   8   -64    -37
 -11   -66   -109
 -10   -59     25
  -9   128    138
  -8   591    589
  -7   137    140
```

```
   L    FO     FC

  -6   336   -348
  -5   150    148
  -4    98   -118
  -3   470    400
  -2   335    356
  -1   144    123

H=     6,  K=    4

   0   130   -129
   1   259   -277
   2   361   -303
   3   119    -97
   4    92    -88
   5   122   -134
   6   320   -323
   7   -65      6
 -11   176    170
 -10   132    126
  -9    90    -66
  -8   210    203
  -7   156    152
  -6   260    272
  -5   -54    -75
  -4   -53     -1
  -3   124   -119
  -2   163    167
  -1    91    -95

H=     7,  K=    4

   0   166   -164
   1   332   -348
   2   233   -226
   3   304   -315
   4   116    131
   5   213   -201
 -10   106    -98
  -9   315    319
  -8   119     81
  -7   -59     90
  -6   -55    -21
  -5   -55    -16
  -4   204   -232
  -3   117    -92
  -2   -56    -48
  -1   463   -467

H=     8,  K=    4

   0   220   -216
   1   187    179
   2   265   -260
   3   129   -130
  -9   119     85
  -8   130   -108
  -7   243   -255
  -6   114   -102
  -5   102    124
  -4   293   -298
  -3   -58     12
  -2   378   -403
  -1    90    -41

H=     9,  K=    4

   0   -61     -9
  -6   110    103
  -5   192   -202
  -4   -60     15
  -3   131   -121
  -2   158    149
  -1   -64    -93

H=     0,  K=    5

   1   287   -285
   2   117    130
   3   406   -386
   4  1537   1483
   L     FO     FC         L     FO     FC         L     FO     FC         L     FO     FC

   5    299   -279        -6    302   -324         2    228   -241
   6    288    275        -5    -49     41         3    167    165      H=     2,  K=    6
   7    156    178        -4    547   -546         4    -59    -38
   8    272    271        -3    828    831         5    182    205         0    625    600
   9    174    169        -2    549    562       -10    -64     -7         1    138   -128
  10    -61     82        -1    780    759        -9    158   -154         2    318   -327
  11    134    153                                -8    -60     -2         3    261    239
                      H=     4,  K=    5          -7    151   -157         4    270    240
H=     1,  K=    5                                -6    207    206         5    -51     58
                         0    -47     40          -5    337   -347         6    -53    -72
   0    733   -683         1     85    -91        -4     87    -72         7    -56    -80
   1   1186   1127         2    889   -916        -3    354   -354         8     77    -57
   2    289   -270         3    200    198        -2    177   -164         9    246   -248
   3    -48     52         4    182   -189        -1    101   -102        10    204    198
   4    537    515         5    -55     45                                -12    -67    -86
   5    583    584         6    619   -617     H=     8,  K=    5         -11    254   -253
   6     95     80         7    -59      9                                -10    -61     89
   7    118     94         8    278   -299         0    285    292        -9    -59    -26
   8     98     81         9    159   -170         1     97    -76        -8    -58    -60
   9    -58   -127       -12    -69    -74         2    194    207        -7    -54     24
  10    -60     -1       -11    217   -205         3    -62     29        -6    194   -187
  11    -62     -8       -10    449    438        -8    249   -249        -5    -48    -17
 -12    -66     65        -9     94     85        -7    130   -116        -4   1109   1124
 -11    362   -364        -8    -58     41        -6    305   -318        -3    596    557
 -10    214    217        -7     88     86        -5    -60    -15        -2    858   -791
  -9    226    218        -6    575    576        -4    -59     75        -1    123    -95
  -8    165   -164        -5    -52     74        -3    241   -241
  -7    744   -742        -4    403    412        -2    103   -113     H=     3,  K=    6
  -6    193   -196        -3    564    561        -1    -58    -27
  -5    211   -219        -2    420    406                                 0    -47     29
  -4    841   -837        -1    807    825     H=     9,  K=    5           1    503   -513
  -3    412    384                                                         2    -47     80
  -2    275    250     H=     5,  K=    5           0    -62     13         3    528    511
  -1    931   -888                                -6    109   -109         4    330   -333
                         0     75     82          -5    120    -94         5    426   -430
H=     2,  K=    5         1    -52    -88        -4    -61    -59         6    487   -499
                         2    234   -234        -3    207    208         7    213    199
   0    532   -501         3    308   -309        -2    -64    -24         8    165   -188
   1    198   -191         4    -56     59        -1    173    156         9    -61     -1
   2    189    169         5    255   -247                                 10    217   -191
   3    321    291         6    220   -217     H=     0,  K=    6         -12    -68    -24
   4    -48     52         7    132   -110                                -11    133    112
   5    418    410         8    200   -192         0    252   -244       -10    294   -288
   6    -53     -6       -11    132    126         1    465   -448        -9    105   -126
   7    293   -292       -10    -63     75         2    148    156        -8    235    267
   8    -57    -22        -9    157    154         3   1181   1136        -7    560    574
   9    203    198        -8    252    253         4    385   -358        -6    637    644
  10    -62    -58        -7    265    279         5    753    703        -5     81     27
 -12    128    -75        -6    339    344         6    123    120        -4    577    570
 -11    139   -110        -5    -50      5         7    625    621        -3    -47     -8
 -10    205   -219        -4    225    232         8    295   -297        -2   1352   1339
  -9    -60     28        -3    165    189         9    318    296        -1     71     48
  -8    220   -215        -2    546    532        10    -60    -46
  -7    294   -318        -1    901   -909        11    -64    -74     H=     4,  K=    6
  -6     84     99
  -5    341   -322     H=     6,  K=    5      H=     1,  K=    6           0    171   -158
  -4    108    -57                                                         1    123    147
  -3    293   -275         0    166   -181         0    144   -134         2    168   -154
  -2    737    725         1    174    178         1    961   -912         3    759   -751
  -1    798   -772         2    137   -144         2    205    231         4    -53    -30
                         3    304   -315         3    884    810         5    355   -332
H=     3,  K=    5         4    104     98         4    926    887         6    -56    -16
                         5    130   -128         5    434   -427         7    383   -367
   0    142   -137         6    119   -140         6    634    618         8     95    124
   1    187   -176       -11    -67     57         7    276   -273         9    -67   -113
   2    313    350       -10    109     94         8    119   -122       -11    125    106
   3    137    144        -9    155    137         9    -59     66       -10    148    158
   4    312    328        -8    -59    -81        10     95   -113        -9    452    469
   5    603   -595        -7    186    197        11    145   -159        -8    -58    -13
   6    -55    -47        -6    120    151       -11    -65     89        -7    535    541
   7    -56     -7        -5     83     64       -10    435   -421        -6    -53     14
   8    283    280        -4    419   -426        -9    210   -241        -5    917    921
   9    328   -326        -3    338    350        -8    -57    -25        -4    189   -188
  10    113   -141        -2    446   -453        -7    251    244        -3    113    124
 -12    -65    -37        -1    285   -307        -6    423   -431        -2    119   -106
 -11    -65    -93                                -5    702   -660        -1    427    442
 -10    342   -331     H=     7,  K=    5          -4     97    -82
  -9    120   -117                                -3    231    235     H=     5,  K=    6
  -8    121    146         0    -55    -15        -2    -50     59
  -7    387    396         1    -55    -35        -1    477    433         0     94    -81
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```
    L    FO     FC

    1   -51    -39
    2    67    -93
    3   -54     33
    4   389   -373
    5   118    122
    6   -58    -50
    7   -60      9
    8   -69   -133
  -11   -64     57
  -10   238    232
   -9    97    -96
   -8   226    226
   -7    91   -109
   -6   140    146
   -5   -52    -45
   -4   -52     30
   -3   150   -162
   -2   178    199
   -1   -50    -77

H=     6,  K=    6

    0   138    130
    1   187   -183
    2   211    232
    3   -57    -70
    4   123   -116
    5   -60     32
    6   251    250
  -11   244    261
  -10   171   -179
   -9   165   -170
   -8   190    190
   -7   -57     31
   -6   343   -350
   -5    78     34
   -4   213    201
   -3   316   -299
   -2   219   -239
   -1   366   -366

H=     7,  K=    6

    0   -55    -59
    1   100    -70
    2   -58     -4
    3   229    231
    4   278    278
    5   -64     14
  -10   -64    -42
   -9   159   -158
   -8   397   -393
   -7   153    134
   -6   307   -313
   -5   -56    -75
   -4   535   -548
   -3   -55     -7
   -2   520   -535
   -1   392    401

H=     8,  K=    6

    0   163    165
    1   170    140
    2   -62    -30
    3   157    149
   -8   -64     60
   -7   395   -413
   -6   -61     28
   -5   236   -238
   -4   207    197
   -3   167   -174
   -2   -58     52
   -1   -59     92

H=     9,  K=    6

    0   -63      7
   -6   -62    -17
   -5   -64     75
```

```
    L    FO     FC

   -4   -63    -17
   -3   -62    -53
   -2   159    178
   -1    98    109

H=     0,  K=    7

    1  1321   1344
    2   864    826
    3  1290   1208
    4   436    412
    5   119   -105
    6   273    260
    7    91    -51
    8   -57    -58
    9   226   -245
   10   157    151
   11   201   -205

H=     1,  K=    7

    0   151   -164
    1   183   -192
    2   179   -179
    3   319    283
    4   227    221
    5   310    315
    6   604   -591
    7   111    -87
    8   189    177
    9   269    276
   10   240   -234
   11   103   -105
  -11   -62    -12
  -10   116   -119
   -9   204   -213
   -8   127    142
   -7   190   -193
   -6   768    751
   -5   -50     15
   -4   602    582
   -3   869   -829
   -2  1088   1039
   -1   365    325

H=     2,  K=    7

    0   359   -324
    1   726    697
    2   371    380
    3   434   -458
    4   -48     30
    5   -50     61
    6    86    110
    7   491   -478
    8   226    232
    9   143   -142
   10   -64    -60
  -12   -66     -3
  -11   -63    -37
  -10   423   -423
   -9   309    297
   -8   151    173
   -7   -55    -12
   -6   281   -265
   -5   556    578
   -4   331    333
   -3   117   -110
   -2   295    299
   -1   109    -89

H=     3,  K=    7

    0   959   -966
    1   283    260
    2   346   -337
    3   186   -183
    4   903   -899
    5   114   -111
    6   281   -290
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    L    FO     FC

    7   -55     86
    8   -58    -65
    9   -62    -60
  -12   269    236
  -11   -64      8
  -10    89    -83
   -9   -58     35
   -8   299    297
   -7   117    129
   -6   331    342
   -5   529    525
   -4   -48     19
   -3   -47     36
   -2   280    291
   -1   928    893

H=     4,  K=    7

    0    83    -88
    1   714   -699
    2   154   -160
    3   225   -216
    4   337   -399
    5   -56     -1
    6    65     30
    7   169    124
    8   298   -300
    9   232    225
  -11   352    347
  -10   -63     72
   -9   117    125
   -8   450    449
   -7   183   -170
   -6   130    128
   -5   -51    -13
   -4   184    172
   -3  1135  -1177
   -2   878    857
   -1   684   -658

H=     5,  K=    7

    0   131    128
    1   110    -90
    2   -53    -57
    3   344   -348
    4   269    259
    5   -59     91
    6   -61    103
    7   331   -329
    8   198    209
  -11   189    179
  -10   -64     79
   -9   132    135
   -8   495   -495
   -7   200    195
   -6   228   -240
   -5   198    213
   -4   498   -495
   -3   -51    -33
   -2   405   -395
   -1   306   -296

H=     6,  K=    7

    0   124   -131
    1   310    302
    2   -57    -83
    3   144    152
    4   -57    -23
    5   329    326
    6   123   -110
  -10   -64    -56
   -9   -60    -13
   -8   161    151
   -7   278   -271
   -6    81     67
   -5   337   -325
   -4   370   -380
   -3   -53     25
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```
    L    FO     FC

   -2   242   -246
   -1   227   -222

H=     7,  K=    7

    0   168    169
    1   142   -159
    2   357    369
    3   108   -104
    4   340    344
    5   217    231
  -10   140   -127
   -9   -63    -56
   -8   283   -277
   -7   158   -154
   -6   -58     -2
   -5    81    -25
   -4   240   -244
   -3   461   -483
   -2   438    451
   -1   248    255

H=     8,  K=    7

    0    99   -119
    1   214    209
    2   102    123
    3    97    -94
   -8   137   -113
   -7   -62     26
   -6   120   -127
   -5   264    258
   -4   169   -161
   -3   252    251
   -2   161    160
   -1   193    195

H=     9,  K=    7

   -6   112    130
   -5   -62     56
   -4   127    125
   -3   -62    -13
   -2   -62     35
   -1   -64     22

H=     0,  K=    8

    0   284    320
    1   739    729
    2  1357   1302
    3   829   -790
    4   -48     18
    5    83    -76
    6   -52     12
    7   308   -277
    8   180    177
    9   198   -207
   10   498   -496
   11   -63     57

H=     1,  K=    8

    0   295   -282
    1   164   -149
    2   818   -799
    3   104    -71
    4   489    448
    5   100   -124
    6   303   -292
    7   388   -383
    8   -56      2
    9   371   -356
   10   -61     16
   11   211   -206
  -11   -64     18
  -10   -60    -18
   -9   -59     80
   -8   -59    -20
   -7   233    216
   L    FO     FC      L    FO     FC      L    FO     FC      L    FO     FC

  -6   604    588   H=    5, K=     8     -2   113    -96    -11   114    107
  -5   510    523                         -1   153   -157    -10   128    151
  -4   135   -159      0   292    295                         -9   200   -211
  -3   601    577      1   226   -222   H=    0, K=     9     -8   311    330
  -2   260    248      2   145   -160                         -7   538   -536
  -1  1101   1055      3   119   -115      1    90    107     -6   -54     47
                       4   311    317      2   573   -543     -5   380   -384
H=    2, K=     8      5   385    391      3   320    334     -4   287    289
                       6   112   -105      4   940   -948     -3   915   -907
   0   185    195      7   101    -90      5   356   -354     -2   330   -316
   1   106    116    -11   -66     75      6   679   -644     -1   329   -327
   2   577   -564    -10   143    159      7   441    443
   3   168   -152     -9   -62     43      8   860   -861   H=    4, K=     9
   4   294   -293     -8   -59    -74      9   362   -381
   5    78    -59     -7   440   -432     10   -62    -95      0   -49     89
   6   293   -277     -6   -55      0     11   -63    -12      1   758   -750
   7   251    266     -5   163   -139                          2   687    679
   8   382   -374     -4   147   -150   H=    1, K=     9      3   -51     43
   9   115    -96     -3   749   -750                          4   435    427
  10   117     75     -2    86     77      0  1053   1005      5   209   -202
 -11   -64    -31     -1   225   -220      1   772   -738      6   528    513
 -10   -61     79                          2   217   -199      7   240   -251
  -9   -58    -58   H=    6, K=     8      3   912   -855      8   259    250
  -8   533    541                          4   361    355    -11   325    322
  -7   -55    -47      0   -53    -41      5   530   -472    -10   366   -364
  -6   170    157      1   -54      4      6   127   -112     -9   -59    -32
  -5   252    250      2   293    285      7   220   -207     -8   434   -433
  -4   897    875      3   -56     -8      8    82     75     -7   302    306
  -3   156   -148      4   -57     51      9   265   -253     -6   669   -688
  -2   145   -163      5   104    -59     10   102    -69     -5   283   -290
  -1   640   -629      6   166    157     11   -64     86     -4   714   -698
                     -10   223   -253    -11   265    259     -3   464   -458
H=    3, K=     8     -9   -60    -15    -10   183    158     -2   -48     57
                      -8   294   -314     -9   304    338     -1   -47     29
   0   210    207     -7   268    265     -8   301   -300
   1   362   -372     -6   419   -418     -7   663    653   H=    5, K=     9
   2   370   -349     -5   -56    -30     -6   220    227
   3   641   -632     -4   217   -214     -5    95     68      0   214    217
   4   260    256     -3   168    170     -4   207   -165      1   217    204
   5   517   -501     -2   177   -198     -3   -48     17      2   384   -379
   6   101     87     -1   -53     17     -2   252   -240      3   541    530
   7   -57     47                         -1   313   -287      4   -56    -47
   8   197    193   H=    7, K=     8                          5   245    247
   9   190   -169                       H=    2, K=     9      6   121    137
 -11   272    275      0   137    138                          7   -62    -18
 -10   -60     31      1   242    247      0   -48    -55    -11   100    -93
  -9   380    393      2   287   -299      1   -47      0    -10   -64     73
  -8   365   -367      3   330    341      2   971   -938     -9   354   -346
  -7   524    530      4   -62    -83      3   -47      1     -8   -57    -14
  -6   -52     -1      5   140    133      4   119    107     -7   293   -284
  -5   100     56     -9   305   -315      5   237   -243     -6   255   -253
  -4   824   -816     -8   177    184      6    87    -80     -5   -54     89
  -3   -48     44     -7   195   -201      7   221    223     -4   407    414
  -2   350   -336     -6   202    196      8   -56      1     -3    90   -105
  -1   220   -225     -5   -55     15      9   153   -160     -2   681   -689
                      -4   242    227     10   163    171     -1   385    393
H=    4, K=     8     -3   -57    -13    -11   -64     42
                      -2   -58     -5    -10   198    207   H=    6, K=     9
   0   577   -579     -1   320    316     -9   -57    -14
   1   363    385                         -8   110   -107      0   207    194
   2   768   -771   H=    8, K=     8     -7   -56     20      1   -54    -14
   3   233    213                         -6   -52    -27      2   326    339
   4    92   -111      0   324    331     -5   -51     72      3   208    201
   5   -57     64      1   200   -206     -4   239   -242      4   -61    113
   6   -59     21      2   162    173     -3   159    160      5   151    132
   7   321    308      3    99    -63     -2   184   -202      6   107   -131
   8    94    106     -8   -64    -80     -1   507    434    -10   238   -219
   9   -66    -87     -7   207    195                         -9   172   -151
 -11   148   -138     -6   160    161   H=    3, K=     9     -8   164    137
 -10   323    343     -5    94     36                         -7    88     76
  -9    98   -108     -4   253    255      0   379   -375     -6   -57     28
  -8   -60    -65     -3   -56     70      1   201   -197     -5   -54    -19
  -7   167   -171     -2   281    289      2   136   -150     -4   384    379
  -6   299    298     -1   -59     30      3    99    -78     -3   156   -163
  -5   747   -771                          4   402   -399     -2   -53    -24
  -4   761   -768   H=    9, K=     8      5   357    350     -1   198    205
  -3   -49     33                          6   183    187
  -2   127   -108     -5   182    172      7   347    360   H=    7, K=     9
  -1   -48    -51     -4    94    100      8   307   -313
                      -3   368    381      9   320    320      0   -58     63
   L    FO     FC

   1   187    192
   2   347    364
   3   209   -196
   4   114    -93
  -9   160    157
  -8   190   -182
  -7   216    218
  -6    96    -72
  -5   387    396
  -4   128    131
  -3   303    285
  -2   282    287
  -1   121    120

 H=    8,  K=    9

   0   214   -216
   1   156    143
   2   193   -192
  -8   214    218
  -7   101    -92
  -6   278    273
  -5   258    266
  -4    93     97
  -3   -61     25
  -2   169    183
  -1   -61     92

 H=    9,  K=    9

  -5   103     82
  -4   190    180
  -3   -64    -75
  -2   -66   -106
  -1    91    -83

 H=    0,  K=   10

   0  1261  -1229
   1   -94     62
   2   205   -191
   3   958   -944
   4   551   -555
   5   603   -604
   6   -53     31
   7   442   -437
   8   132    119
   9   406   -423
  10   -61    -40
  11   120    -84

 H=    1,  K=   10

   0  1153  -1103
   1    82    -84
   2   528   -495
   3   -47    -18
   4   146   -178
   5   487    479
   6   190   -182
   7   132    118
   8   -56    -58
   9   207    210
  10   111    -90
 -11    96     74
 -10   385    389
  -9   296   -303
  -8   458    455
  -7   513   -511
  -6   302    284
  -5   128    139
  -4   260    251
  -3  1156  -1086
  -2   169   -156
  -1   -47     20

 H=    2,  K=   10

   0   -47     39
   1   827   -821
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```
   L    FU     FC

   2   674    653
   3   -47     22
   4   232    249
   5   -51     61
   6   152    159
   7   149   -166
   8   328    333
   9   413    423
  10   -64     26
 -11   240    250
 -10   145   -172
  -9    85     38
  -8   351   -348
  -7   161   -162
  -6    94   -112
  -5   442    421
  -4   504   -486
  -3   388   -411
  -2   194   -151
  -1   128    -96

 H=    3,  K=   10

   0   168   -182
   1   859    803
   2   114   -111
   3   347    335
   4   -53     40
   5   283    277
   6   464    466
   7   181    183
   8   236    225
   9    99     85
 -11   105    -76
 -10   104   -107
  -9   179   -188
  -8   142    156
  -7   307   -318
  -6   585   -599
  -5   176   -170
  -4    99   -110
  -3   -48    -36
  -2   901   -918
  -1   305    283

 H=    4,  K=   10

   0   123    122
   1   204    200
   2   323    318
   3   383    373
   4   209    206
   5   384    385
   6   222   -219
   7   162    164
   8   181    165
 -11   112     68
 -10    90    -85
  -9   418   -424
  -8   136   -140
  -7   394   -393
  -6   390    394
  -5   817   -822
  -4   184    178
  -3   260   -279
  -2   570    579
  -1   237    228

 H=    5,  K=   10

   0   -51     -2
   1   287    287
   2   414    426
   3   361   -373
   4   254    258
   5   -58     47
   6   105   -124
   7   137   -136
 -11   -64    -39
 -10   277   -273
```

```
   L    FO     FC

  -9   262    258
  -8   250   -297
  -7   -57     40
  -6   237   -231
  -5   381    383
  -4   -52     48
  -3   -51     39
  -2   281    284
  -1   294   -298

 H=    6,  K=   10

   0    94    -75
   1   483    486
   2   197   -193
   3   -56    -24
   4   196   -208
   5   -62     45
   6   -63    -75
 -10   -64     30
  -9   -62    -20
  -8   -57      8
  -7   211   -206
  -6   -57    106
  -5   487    486
  -4   121    122
  -3   137   -107
  -2    80    -29
  -1   228    209

 H=    7,  K=   10

   0   -56    -58
   1   162   -158
   2   144    151
   3   137   -145
   4   232   -233
  -9   148    147
  -8   334    344
  -7   -59     44
  -6   144    146
  -5    90     87
  -4   317    313
  -3   -56    -59
  -2   485    492
  -1   212   -208

 H=    8,  K=   10

   0   -62     76
   1   204   -208
   2   -63    -14
  -8   163   -161
  -7   133    130
  -6   -62     35
  -5   267    288
  -4   153   -150
  -3   -60     99
  -2   128   -130
  -1   -61    -60

 H=    9,  K=   10

  -4   -62    -65
  -3   -66    103
  -2   132   -160

 H=    0,  K=   11

   1  1237  -1220
   2   509    489
   3   889   -864
   4   391    352
   5   126   -121
   6    81    -87
   7   -56    -21
   8   188    204
   9   385    379
  10   -61    -43
  11   236    246
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```
   L    FO     FC

 H=    1,  K=   11

   0   784   -769
   1   172    166
   2   448   -417
   3   346    317
   4   393    386
   5   455   -460
   6   252    240
   7   432    412
   8   472    483
   9   104   -111
  10   312    297
 -11   -65    -32
 -10   -63     31
  -9    91    -85
  -8   237   -250
  -7   170    163
  -6   508   -505
  -5   139   -147
  -4   645   -627
  -3   325    333
  -2   559   -552
  -1   633   -597

 H=    2,  K=   11

   0   211   -163
   1   136    170
   2   721   -704
   3   281    274
   4   484    473
   5   527    515
   6   319   -328
   7   190    205
   8   300    290
   9   211    187
  10   135    131
 -11   -64     26
 -10   379    370
  -9   411   -437
  -8   180   -183
  -7   339   -336
  -6   402    388
  -5   334   -334
  -4   261   -257
  -3   332   -329
  -2   389   -366
  -1   223    202

 H=    3,  K=   11

   0   422    417
   1   516    522
   2   987    981
   3   571   -566
   4   398    397
   5   -54    -14
   6   174    182
   7   109     96
   8   -60     67
   9   -64     39
 -11   105   -110
 -10   392   -410
  -9   167    178
  -8   405   -400
  -7   237   -232
  -6   104   -110
  -5   210   -225
  -4   141   -130
  -3   502    483
  -2   734    727
  -1   779   -783

 H=    4,  K=   11

   0   -49     18
   1   859    857
   2   230   -226
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L	FO	FC
3	131	114
4	93	70
5	91	101
6	99	99
7	215	-210
8	103	91
-11	155	-169
-10	-61	-24
-9	273	-267
-8	-58	36
-7	207	214
-6	-55	-21
-5	407	387
-4	-51	-1
-3	440	428
-2	-48	2
-1	588	587
H=	5, K=	11
0	265	243
1	-53	19
2	-54	-20
3	383	375
4	103	-89
5	-58	-48
6	270	-288
7	90	64
-11	-67	48
-10	-65	61
-9	-61	23
-8	161	158
-7	-57	-44
-6	281	277
-5	81	-79
-4	367	387
-3	104	101
-2	78	55
-1	287	269
H=	6, K=	11
0	298	302
1	119	-103
2	-56	-35
3	183	-181
4	-58	-12
5	306	-314
6	-64	-18
-10	133	102
-9	190	200
-8	101	-94
-7	145	134
-6	-57	77
-5	272	288
-4	331	350
-3	79	-7
-2	133	-134
-1	-56	-80
H=	7, K=	11
0	158	-178
1	99	60
2	348	-350
3	-59	-41
4	243	-249
-9	-63	24
-8	149	128
-7	275	279
-6	153	129
-5	268	-274
-4	87	-97
-3	207	211
-2	271	-272
-1	181	-175
H=	8, K=	11
0	-60	-40

L	FO	FC
1	176	-178
2	174	-193
-7	-65	-56
-6	-62	-62
-5	217	-229
-4	-59	-23
-3	199	-175
-2	-60	63
-1	230	-223
H=	0, K=	12
0	1628	-1542
1	227	308
2	1240	-1265
3	533	492
4	-48	-36
5	464	440
6	-55	49
7	259	251
8	137	146
9	218	214
10	365	378
11	-65	43
H=	1, K=	12
0	-49	-65
1	328	-326
2	927	877
3	-48	56
4	124	132
5	-50	37
6	329	327
7	302	309
8	138	144
9	319	323
10	124	-136
-11	-64	44
-10	314	-305
-9	91	-117
-8	152	-148
-7	96	113
-6	-54	-44
-5	641	-662
-4	378	-385
-3	292	-302
-2	780	764
-1	855	-840
H=	2, K=	12
0	539	499
1	138	127
2	-49	-36
3	258	253
4	-51	43
5	158	145
6	306	308
7	-55	-42
8	125	127
9	-61	29
10	-66	101
-11	-65	9
-10	-63	-69
-9	226	-234
-8	133	-133
-7	-59	-58
-6	237	-228
-5	734	725
-4	-51	-31
-3	105	-134
-2	257	242
-1	627	623
H=	3, K=	12
0	493	484
1	284	283
2	416	411

L	FO	FC
3	462	454
4	510	-490
5	236	249
6	-55	-18
7	116	-128
8	215	-209
9	160	-151
-11	-65	-63
-10	101	-63
-9	251	-231
-8	318	342
-7	-58	69
-6	168	175
-5	263	-255
-4	625	603
-3	214	225
-2	-48	11
-1	988	982
H=	4, K=	12
0	695	697
1	-53	-71
2	388	380
3	465	-469
4	86	-78
5	522	-515
6	148	-142
7	-61	6
8	348	-362
-11	-66	78
-10	-63	-9
-9	324	316
-8	-61	-84
-7	184	159
-6	-57	-80
-5	183	194
-4	639	644
-3	281	289
-2	394	388
-1	-50	-44
H=	5, K=	12
0	271	-280
1	100	-118
2	298	-298
3	-55	-29
4	-54	-12
5	211	-204
6	102	-115
7	-65	-96
-10	211	209
-9	220	-214
-8	-60	13
-7	424	417
-6	-58	53
-5	170	182
-4	-54	-65
-3	218	219
-2	251	-254
-1	213	222
H=	6, K=	12
0	87	-62
1	86	75
2	188	-195
3	-59	-88
4	-61	-91
5	119	112
6	-63	-55
-10	129	136
-9	210	224
-8	180	178
-7	319	-291
-6	-56	11
-5	-56	45
-4	222	213
-3	261	-265

L	FO	FC
-2	180	-168
-1	182	-191
H=	7, K=	12
0	218	-217
1	415	-408
2	179	183
3	-61	-60
4	-63	-12
-9	-64	73
-8	-59	43
-7	109	84
-6	222	-219
-5	-60	17
-4	131	-132
-3	158	-169
-2	-58	81
-1	109	-105
H=	8, K=	12
0	206	-210
1	-62	-9
2	-64	45
-7	-63	-46
-6	183	-193
-5	113	-128
-4	-62	-54
-3	-60	38
-2	345	-353
-1	109	72
H=	0, K=	13
1	143	189
2	529	514
3	475	-469
4	356	344
5	342	339
6	836	820
7	-57	-67
8	181	186
9	147	126
10	174	171
H=	1, K=	13
0	691	-673
1	-47	46
2	351	343
3	914	890
4	547	-546
5	274	253
6	184	186
7	-57	37
8	204	217
9	142	-150
10	110	-119
-11	97	-99
-10	163	-154
-9	564	-584
-8	196	182
-7	99	-88
-6	146	-131
-5	135	-142
-4	77	-77
-3	-48	20
-2	463	436
-1	981	952
H=	2, K=	13
0	393	399
1	151	171
2	517	487
3	176	-171
4	-52	-68
5	-54	34
6	166	-146

```
   L    FO     FC

   7   139    138
   8   299   -298
   9   -62    -37
 -11   -66    -43
 -10   107   -110
  -9   -60     35
  -8   211   -208
  -7   206   -220
  -6   155    128
  -5    96     76
  -4   385    368
  -3   -50    -19
  -2   452    442
  -1   112    115

 H=     3,  K=   13

   0   229    224
   1   609    587
   2   -50    -35
   3   555   -585
   4   297    287
   5   128   -141
   6   180   -181
   7   431   -449
   8   146    125
   9   207   -234
 -11   -67    -93
 -10   -65     80
  -9   116    108
  -8   106   -123
  -7   -58     -8
  -6   -56    -36
  -5   775    764
  -4   -51    -17
  -3   508    517
  -2   255    259
  -1   416    407

 H=     4,  K=   13

   0   476   -455
   1   311    311
   2   175   -182
   3   -55    -46
   4   419   -407
   5   336    339
   6   290   -279
   7   194   -202
   8   -66    -73
 -11   222   -206
 -10   199    217
  -9   208    216
  -8   482    494
  -7   126   -117
  -6   214    223
  -5   114    117
  -4   379    371
  -3   198    188
  -2   184    193
  -1   183   -173

 H=     5,  K=   13

   0   243   -245
   1   362   -369
   2   153    162
   3   -56     29
   4   112     91
   5   139   -139
   6   174   -196
   7   -63    -29
 -10   -65     -2
  -9   252    250
  -8   -59     51
  -7   181   -181
  -6   129    130
  -5   218    209
  -4   150   -198
  -3   341   -333
```

```
   L    FO     FC

  -2   245    246
  -1   202   -213

 H=     6,  K=   13

   0   288   -302
   1   211   -199
   2   -56     49
   3   142   -143
   4   138   -131
   5   -63     10
  -9   -62    -32
  -8   -61     37
  -7   -60     -3
  -6   -58    -67
  -5   105   -101
  -4   116   -119
  -3    77    -33
  -2   380   -393
  -1   -56    -11

 H=     7,  K=   13

   0   -61    -93
   1   137    114
   2   140   -148
   3   -60      6
   4   -64     61
  -8   -63    -53
  -7   108   -107
  -6   -61    -91
  -5   484   -486
  -4   -59    -66
  -3   174   -152
  -2   -56     -6
  -1   279   -291

 H=     8,  K=   13

   0   -60     37
   1   -62      6
  -7   -64     12
  -6   238   -241
  -5   149   -143
  -4   -62    -63
  -3   165    161
  -2   135    140
  -1   -64   -110

 H=     0,  K=   14

   0   411    441
   1   490    566
   2   485    552
   3   220    239
   4   608    598
   5   402    399
   6   125   -136
   7   618    612
   8   300   -304
   9   113    125
  10   203   -188

 H=     1,  K=   14

   0   617    577
   1   721    682
   2   292    284
   3   198   -196
   4   790    775
   5    89    -84
   6   137    136
   7   -55      2
   8   184    168
   9   204   -196
  10   -64   -103
 -11   123   -148
 -10   124   -139
  -9   115   -122
  -8   392   -390
```

```
   L    FO     FC

  -7   105    123
  -6   -55    -31
  -5   326    321
  -4   205   -226
  -3   618    621
  -2   304    295
  -1   412   -388

 H=     2,  K=   14

   0   -47    -42
   1   300    311
   2   199    185
   3   243    245
   4   -53    -47
   5   131    124
   6   299   -293
   7   306   -315
   8   157    138
   9   -65   -131
 -11   190   -183
 -10   -62     37
  -9   105    106
  -8   123    139
  -7   309   -307
  -6   128   -131
  -5   265    255
  -4   155   -122
  -3   667    550
  -2   277    275
  -1   398    381

 H=     3,  K=   14

   0   187    194
   1   526   -524
   2   259   -267
   3   317   -315
   4    97    -87
   5   256   -254
   6   387   -391
   7   141   -148
   8   316   -319
   9   140    136
 -11   -67     59
 -10   193    178
  -9   332    343
  -8   103   -102
  -7   112   -109
  -6   413    409
  -5   219    208
  -4   460    448
  -3   301   -278
  -2   143    136
  -1    85    -71

 H=     4,  K=   14

   0   517   -517
   1   239   -225
   2   167   -152
   3   378   -381
   4   124   -117
   5   372   -375
   6   189    171
   7   205   -179
   8   -63     61
 -10   157    172
  -9   185    172
  -8   294    295
  -7   374    382
  -6   392   -378
  -5   125   -120
  -4   242   -244
  -3   383    369
  -2   698   -710
  -1   370   -358

 H=     5,  K=   14
```

```
   L    FO     FC

   0   224   -228
   1   221   -224
   2   439   -473
   3   202    195
   4   -58     41
   5   117    106
   6   119   -120
   7   171    180
 -10   307    287
  -9   253   -265
  -8   -62    -48
  -7   -59     91
  -6   119    141
  -5   390   -386
  -4   141   -113
  -3   -55    -69
  -2   212   -214
  -1   -52     -7

 H=     6,  K=   14

   0   -55     16
   1   -55    -12
   2    97     52
   3    97     72
   4   273    288
   5   -63    -56
  -9   -65     80
  -8   113    -86
  -7   -59     12
  -6   133    121
  -5   188   -198
  -4   121    -61
  -3   -57    -10
  -2   101     95
  -1   441   -444

 H=     7,  K=   14

   0   -60     41
   1   306    300
   2   -63     76
   3   -63     57
  -8   123   -136
  -7   -63    -83
  -6   -61    -69
  -5   -60     18
  -4   166   -157
  -3   117    118
  -2   204   -205
  -1   289    288

 H=     8,  K=   14

   0   -63     30
   1   -63     68
  -6   -64     38
  -5   206   -220
  -4   130    126
  -3   -62     67
  -2   283    275
  -1   -63     31

 H=     0,  K=   15

   1   423    481
   2   301    299
   3   699    681
   4    87     97
   5   278    271
   6   200    192
   7   372   -375
   8   -58      2
   9   143   -148
  10   -63     22

 H=     1,  K=   15

   0   444    446
   1   149   -163
   L    FO     FC

   2   175    162
   3   181    150
   4   352   -355
   5   -53     46
   6   224   -229
   7   104     93
   8   489   -495
   9   149    155
  10   -63     -7
 -10   -65    -79
  -9   -62    -55
  -8   112    107
  -7   226   -217
  -6   -57    -97
  -5   104   -103
  -4  1086   1074
  -3   134   -149
  -2   171    181
  -1   202    200

H=     2,  K=   15

   0    71     -6
   1   655   -636
   2   -50     41
   3   118   -134
   4   -53     13
   5   552   -556
   6   251    239
   7    95   -107
   8   132   -103
   9   115    -87
 -10   126    -98
  -9   -61    -39
  -8   -60     55
  -7   634    621
  -6   -58    108
  -5    90    -86
  -4   195    187
  -3   422    411
  -2   186   -174
  -1   243    225

H=     3,  K=   15

   0   285   -273
   1   132   -111
   2   742   -735
   3   -54    -54
   4   123   -103
   5   -56     78
   6   232   -222
   7   190   -189
   8    93   -100
 -10   481    485
  -9   116     85
  -8   309    330
  -7   219    229
  -6   -57    -49
  -5    92    114
  -4   176    187
  -3   293   -279
  -2   522   -515
  -1   390    390

H=     4,  K=   15

   0   -53     11
   1   510   -513
   2   125   -141
   3   -54     19
   4   133   -112
   5   142   -137
   6   -60     27
   7   171    192
 -10   -64    -10
  -9   142    105
  -8    92     87
  -7   180    180
  -6   107    105
```

```
   L    FO     FC

  -5   234   -228
  -4   -54      7
  -3   442   -452
  -2   243    224
  -1   678   -687

H=     5,  K=   15

   0   350   -356
   1    99    -73
   2   419    434
   3   -57    -85
   4   191   -185
   5   -60     56
   6   347    333
 -10   135    -97
  -9   -63      3
  -8   116     93
  -7   -56    -11
  -6   112   -112
  -5   157    159
  -4   407   -405
  -3   131   -150
  -2   258   -259
  -1   -53     23

H=     6,  K=   15

   0   -55    -12
   1   106    -49
   2   165    172
   3   128    132
   4   161   -157
   5   213    200
  -9   258   -259
  -8   -61    -20
  -7    97    -60
  -6   -58    -45
  -5   167   -159
  -4    91    -76
  -3   240   -227
  -2   -56     52
  -1   470    459

H=     7,  K=   15

   0   361    366
   1   -63     63
   2   203    204
   3   -63    -63
  -8   -64    -58
  -7   -63    -81
  -6   292   -283
  -5   -61     47
  -4   382    371
  -3   -60     92
  -2   132    124
  -1   -60    -30

H=     8,  K=   15

   0   -63    -48
  -6   -62    -21
  -5   171    146
  -4   -63      9
  -3   179    210
  -2   -64    -52
  -1   394    391

H=     0,  K=   16

   0   743    696
   1   225   -254
   2   370    381
   3   347   -332
   4   608    593
   5   213   -212
   6   164    163
   7   420   -407
   8    85    -89
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```
   L    FO     FC

   9   -62     92
  10   -66   -100

H=     1,  K=   16

   0   -48     50
   1   451    456
   2   364   -365
   3   261   -261
   4    98    -95
   5   -55     79
   6   -53     -1
   7   353   -326
   8   -58    -17
   9   132   -143
 -10   132    115
  -9   127    113
  -8   400    407
  -7   264    275
  -6   201    181
  -5   563    559
  -4   141    130
  -3   530    498
  -2   385   -377
  -1   294    276

H=     2,  K=   16

   0   342   -343
   1   238   -219
   2   134   -126
   3    99   -108
   4   457   -425
   5   189   -181
   6   534   -519
   7    94     19
   8   -58     11
   9    90     70
 -10   -63      8
  -9    96     89
  -8   266    270
  -7   315    314
  -6   353    327
  -5   118    -95
  -4   111   -129
  -3   242   -219
  -2   625    593
  -1   222    179

H=     3,  K=   16

   0   393   -370
   1   387   -380
   2    84    -92
   3   663   -659
   4   218   -218
   5    95   -102
   6   303    313
   7   296   -287
   8   242    236
 -10   -65     42
  -9   296    303
  -8   -60    -86
  -7   -57    -67
  -6   106    107
  -5   286    293
  -4   478   -470
  -3   458   -473
  -2   253   -244
  -1    77    -80

H=     4,  K=   16

   0   547   -560
   1   158    147
   2   -53     29
   3   176    167
   4   208   -198
   5   478    473
   6   -59     20
```

```
   L    FO     FC

   7   114     33
 -10   -65     47
  -9   267   -264
  -8   188    193
  -7   221   -190
  -6   331   -339
  -5   220   -217
  -4   254   -252
  -3   464   -453
  -2   237   -278
  -1   251    263

H=     5,  K=   16

   0   330    393
   1   -56      7
   2   238    230
   3   137    118
   4   153    123
   5   -60     16
   6   145    136
  -9   -63     29
  -8   -62    -67
  -7   202   -214
  -6   224   -214
  -5   203   -201
  -4   277    259
  -3   -58     20
  -2   166    159
  -1   376   -375

H=     6,  K=   16

   0    85    -65
   1   226    233
   2    99    127
   3   105     97
   4   274    259
   5   -63     58
  -9   -65    -75
  -8   253   -257
  -7   -62     -7
  -6   -60     48
  -5   236    231
  -4   218   -205
  -3   -56     85
  -2   -57     65
  -1   292    281

H=     7,  K=   16

   0   174    147
   1   297    293
   2    97    -58
   3   -62     -9
  -7   154   -149
  -6   148    156
  -5    92    -97
  -4   -60     68
  -3   224    215
  -2   218    241
  -1   -61     19

H=     8,  K=   16

   0   -64     53
  -5   105     80
  -4   -63      9
  -3   -62     42
  -2   233    242
  -1   153   -148

H=     0,  K=   17

   1   130   -179
   2   681   -685
   3   173   -160
   4   232   -223
   5   191    194
   6   977   -949
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L	FO	FC
7	-58	46
8	-60	-63
9	-63	-7
10	204	-201
H=	1, K=	17
0	251	253
1	286	-261
2	184	195
3	820	-810
4	360	-356
5	106	-96
6	208	216
7	241	-232
8	-58	26
9	-62	-51
-10	101	-90
-9	374	354
-8	-60	55
-7	370	365
-6	-57	-1
-5	-55	47
-4	179	191
-3	97	88
-2	159	-159
-1	287	-310
H=	2, K=	17
0	411	-399
1	190	-175
2	351	-344
3	183	-203
4	-54	45
5	-56	-17
6	94	-83
7	183	184
8	-58	39
9	-63	-19
-10	102	114
-9	92	-61
-8	-60	35
-7	175	174
-6	95	-53
-5	-56	69
-4	235	-226
-3	-51	26
-2	226	-236
-1	586	571
H=	3, K=	17
0	197	189
1	221	-213
2	125	-81
3	355	360
4	282	277
5	-57	-58
6	-58	-37
7	439	419
8	-65	-45
-10	129	108
-9	-64	-70
-8	-60	-17
-7	107	-108
-6	241	-233
-5	548	-534
-4	169	168
-3	388	-356
-2	-52	-24
-1	709	-686
H=	4, K=	17
0	421	426
1	253	262
2	-55	-22
3	-56	34
4	439	437

L	FO	FC
5	93	-50
6	280	287
7	-63	-30
-10	-64	-26
-9	-64	0
-8	545	-542
-7	225	-218
-6	347	-347
-5	-56	53
-4	442	-445
-3	-55	43
-2	475	-456
-1	160	-144
H=	5, K=	17
0	243	-238
1	260	269
2	190	176
3	169	150
4	-61	-29
5	195	184
6	-65	25
-9	226	-211
-8	-61	68
-7	-63	-117
-6	149	-132
-5	404	-396
-4	178	-162
-3	392	386
-2	-55	5
-1	-57	-12
H=	6, K=	17
0	391	391
1	-59	-44
2	-59	36
3	-61	-2
4	121	122
-8	112	-121
-7	-63	-89
-6	127	128
-5	-60	-79
-4	138	139
-3	-56	16
-2	189	181
-1	-59	-28
H=	7, K=	17
0	112	-121
1	-63	-73
2	122	-108
-7	290	289
-6	106	-99
-5	330	329
-4	-62	89
-3	174	174
-2	110	-96
-1	438	437
H=	8, K=	17
-4	179	174
-3	-62	-17
-2	105	-71
-1	-64	-50
H=	0, K=	18
0	222	-214
1	543	-615
2	686	-689
3	-71	-18
4	-54	69
5	147	-139
6	-58	-21
7	394	-408
8	-60	-14

L	FO	FC
9	-61	-3
H=	1, K=	18
0	119	145
1	196	-193
2	534	-518
3	-53	35
4	342	-329
5	125	-118
6	307	-305
7	391	395
8	144	-145
9	-63	64
-10	106	85
-9	-65	-69
-8	228	217
-7	102	-126
-6	254	-254
-5	-55	-47
-4	411	426
-3	259	-265
-2	225	-220
-1	535	-537
H=	2, K=	18
0	106	105
1	289	-273
2	96	97
3	91	-91
4	147	-141
5	112	-97
6	296	304
7	-60	43
8	-61	-31
-10	-66	61
-9	94	104
-8	193	-188
-7	-58	-5
-6	260	-270
-5	309	-297
-4	332	-339
-3	203	-196
-2	359	-355
-1	369	-338
H=	3, K=	18
0	335	-312
1	346	346
2	123	120
3	193	177
4	98	94
5	295	273
6	104	91
7	-62	49
8	107	124
-10	-67	-60
-9	264	-264
-8	147	-158
-7	337	-325
-6	311	-317
-5	408	-408
-4	508	-496
-3	134	152
-2	80	-63
-1	247	235
H=	4, K=	18
0	544	524
1	106	-99
2	371	364
3	193	184
4	116	128
5	379	368
6	104	124
7	-65	63
-9	111	-91

L	FO	FC
-8	-62	-19
-7	353	-354
-6	-59	-59
-5	93	-92
-4	563	555
-3	201	-217
-2	136	118
-1	158	-146
H=	5, K=	18
0	-57	51
1	-56	25
2	348	330
3	133	124
4	-60	34
5	141	-134
-9	-64	-38
-8	-64	-36
-7	390	387
-6	220	-226
-5	248	247
-4	110	102
-3	106	119
-2	142	-135
-1	454	449
H=	6, K=	18
0	-58	-4
1	-61	-62
2	179	-162
3	109	113
4	212	-136
-8	150	155
-7	126	140
-6	224	219
-5	96	106
-4	219	218
-3	-56	37
-2	-59	76
-1	292	281
H=	7, K=	18
0	95	110
1	247	-252
2	101	-100
-7	199	201
-6	293	296
-5	-64	25
-4	-59	54
-3	-61	-88
-2	119	113
-1	205	-209
H=	0, K=	19
1	654	-660
2	-63	31
3	562	-611
4	102	-94
5	200	187
6	148	128
7	117	-124
8	226	228
9	135	142
H=	1, K=	19
0	447	-450
1	314	318
2	174	181
3	144	-140
4	-52	-3
5	413	400
6	-57	92
7	-62	-96
8	257	273
9	-64	56

```
   L     FO      FC

  -9     95      63
  -8    151    -134
  -7    -59     -57
  -6    291    -316
  -5    105     106
  -4    557    -548
  -3    -55      79
  -2    438    -422
  -1    313     310

H=      2,  K=   19

   0    -52      18
   1    445     457
   2    411     400
   3    213    -215
   4     83     -97
   5    406     375
   6    131     118
   7    236     229
   8    -63     -58
 -10    -66     -63
  -9    -63     -20
  -8    247     240
  -7    587    -587
  -6    177    -168
  -5    -57     -29
  -4    244     242
  -3    177    -183
  -2    194     193
  -1    322    -301

H=      3,  K=   19

   0    141     122
   1    167    -183
   2    587     564
   3    364     353
   4    297     285
   5    107     -95
   6    239     245
   7    -62     -60
  -9    157    -159
  -8    334    -320
  -7    290     274
  -6    -57     -15
  -5    -60      68
  -4    151    -193
  -3    102    -103
  -2    107     114
  -1    343     336

H=      4,  K=   19

   0    160     143
   1    671     645
   2    135    -134
   3    -58      91
   4    -59     -33
   5    -59       8
   6    -62     -67
  -9    119    -114
  -8    -62      13
  -7    -62      -1
  -6    176     166
  -5    208     209
  -4    -57      -8
  -3    364     348
  -2    120    -117
  -1    291     274

H=      5,  K=   19

   0    169     160
   1    -56       8
   2     87     -46
   3    123    -123
   4    -60     -43
   5    -63      33
  -9    -64       8
```

```
   L     FO      FC

  -8    -65      92
  -7     97      55
  -6    478     473
  -5    117     -96
  -4    266     262
  -3     97      90
  -2    310     279
  -1    106    -113

H=      6,  K=   19

   0    125    -132
   1    -60      59
   2    -60      53
   3    250    -247
   4    -63     -43
  -8    -64     -20
  -7    262     246
  -6    -62       1
  -5    304     312
  -4    -60     -44
  -3    120     110
  -2     87      74
  -1    -60       7

H=      7,  K=   19

   0    181    -174
   1    -65     -80
  -6    185     183
  -5    -65      93
  -4    -62     -60
  -3    166    -173
  -2     89      22
  -1    -61      28

H=      0,  K=   20

   0    223    -224
   1    431     454
   2    -63     -56
   3    372     379
   4    101     102
   5    168     149
   6     87     -65
   7    404     416
   8    -63      61
   9    105     110

H=      1,  K=   20

   0    553     541
   1    -53     -53
   2    262     269
   3     95      87
   4    -54       3
   5    -57     -88
   6    153     149
   7    215     208
   8    -60      40
  -9    -66     -76
  -8    361    -353
  -7    110     -99
  -6    169    -175
  -5    272     277
  -4    119    -122
  -3    526    -525
  -2    146    -166
  -1    -53      33

H=      2,  K=   20

   0    249     254
   1    466     465
   2    -56      12
   3    166     149
   4     81      67
   5    -56     -69
   6    271     262
   7    114     110
```

```
   L     FO      FC

   8    -62      14
  -9    -62       3
  -8    101    -116
  -7    -61      67
  -6    -57      -1
  -5    310    -300
  -4    346    -348
  -3    558     541
  -2     90     -68
  -1    143    -154

H=      3,  K=   20

   0    336     341
   1    309     312
   2    -57      28
   3    115     115
   4    -59      89
   5    126     140
   6    356    -344
   7    -64      89
  -9    168    -172
  -8    -61     -38
  -7    -63     -95
  -6    577     585
  -5    274    -266
  -4    232     219
  -3    270     262
  -2    522     524
  -1    135    -128

H=      4,  K=   20

   0    192     210
   1    276    -278
   2    190     184
   3    226    -218
   4    131     127
   5    198    -193
   6    -63     -59
  -9    281     274
  -8    175    -157
  -7    444     443
  -6    -60      28
  -5    437     447
  -4    219     211
  -3    296     296
  -2    -55     -92
  -1    188     189

H=      5,  K=   20

   0    136    -145
   1    101     102
   2    257    -236
   3    -61     -35
   4    106    -119
   5    100    -116
  -8    125     130
  -7    -63      18
  -6    142     130
  -5    248     245
  -4    -57      26
  -3    -57       8
  -2    -58     -46
  -1    111      96

H=      6,  K=   20

   0    149    -134
   1    238    -215
   2    108    -100
   3    -62      61
  -7    105      84
  -6    -62     -35
  -5    358    -366
  -4    193     186
  -3    -60      22
  -2    -60     -13
  -1    201    -206
```

```
   L     FU      FC

H=      7,  K=   20

   0    116     102
   1    188    -199
  -5    -63     -29
  -4    257    -238
  -3    -61     -27
  -2    296    -308
  -1    138    -149

H=      0,  K=   21

   1    198     222
   2    223     233
   3    401     473
   4    193     201
   5     99    -113
   6    497     504
   7    108     122
   8    338     337
   9    128    -123

H=      1,  K=   21

   0    268     280
   1    303     292
   2    329    -329
   3    454     448
   4    -56      61
   5    306     289
   6    110    -123
   7    156     141
   8    -60     -11
  -9    114    -104
  -8    -61     -43
  -7    423    -408
  -6    507     508
  -5    -57      21
  -4    105     112
  -3    138    -156
  -2    115     130
  -1    138     133

H=      2,  K=   21

   0    145     123
   1    158    -158
   2    612     583
   3    137    -128
   4    284    -286
   5    -57      -8
   6     88      95
   7    143    -142
   8    120    -150
  -9    143     118
  -8    -63      17
  -7    155     154
  -6    164    -150
  -5    132    -106
  -4    262     252
  -3    -56     -44
  -2    102      77
  -1    203     228

H=      3,  K=   21

   0    164    -135
   1    197    -205
   2    218    -206
   3    -58      60
   4    250    -228
   5    260    -247
   6    -62      40
   7    294    -292
  -9    -65      23
  -8    -64      53
  -7    257     250
  -6    103     -79
  -5    282     274
```

```
   L    FO     FC      L    FO     FC      L    FO     FC      L    FO     FC

  -4   -57     17      5   229   -244     -3   242   -250     -7   -63    -21
  -3   199    190      6   152    156     -2   -58    -14     -6   -65   -117
  -2    91    102      7   435   -413     -1   129   -127     -5   206   -178
  -1   235    218      8   -62    -50                          -4   -60     75
                      -9   -66     66   H=     6, K=   22     -3    86     93
H=     4, K=   21     -8   117   -124                          -2   109   -135
                      -7   -63     68      0   -63    104     -1   295   -300
   0   237   -260     -6   191   -185      1   126   -119
   1   232   -231     -5   388    397      2   218    209   H=     4, K=   23
   2    96   -101     -4   169   -209     -6   -63    -75
   3   165    175     -3   -56     15     -5   -64    -96      0   207    204
   4   409   -386     -2   148    158     -4   151   -165      1   433   -426
   5   -60    -13     -1   436    439     -3   -61    -63      2   192    211
   6   262   -277                          -2   -61     79      3   114    109
  -8   324    320   H=     2, K=   22     -1   129   -123      4   240    238
  -7    88     78                                              5   145   -126
  -6   173    102      0    79    -66   H=     7, K=   22     -8   165   -158
  -5   183   -175      1    97     99                         -7   -63    -46
  -4   335    328      2   320   -309     -3   149    149     -6   -60    -27
  -3   183   -180      3   -56     35     -2   114   -110     -5   -60      1
  -2   -55     11      4   348   -349                         -4   -61    -64
  -1   -57    -62      5    98     87   H=     0, K=   23     -3   422   -422
                       6   153   -172                         -2    93    -79
H=     5, K=   21      7   -63    -80      1   309    298     -1   135   -182
                      -9   -66    -35      2   233   -277
   0   246    236     -8   328    307      3   635    680   H=     5, K=   23
   1   262   -258     -7   -60    -14      4   318   -321
   2   -59     15     -6   200    205      5   137   -113      0    93    104
   3   292   -299     -5   259   -250      6   244   -241      1   -61     28
   4   -63     40     -4   290    289      7   -61     44      2   120   -108
  -8   -64    -14     -3   212    212      8   -64    -68      3   -66    107
  -7   -62     61     -2   245    245                         -7   103     22
  -6   280   -275     -1   -55     18   H=     1, K=   23     -6   -62    -43
  -5   -61     62                                             -5   100    -37
  -4   142    127   H=     3, K=   22      0   329    364     -4   249   -242
  -3   -59     20                          1   -55    -85     -3   178    178
  -2   251   -238      0   -57      3      2   -61     85     -2   152   -170
  -1   157   -144      1   251   -243      3   205   -190     -1   -59     58
                       2   240    249      4   -58    -20
H=     6, K=   21      3   317   -322      5   170   -164   H=     6, K=   23
                       4   -60    -44      6   346   -337
   0   290   -297      5   119   -126      7   -62     43      0   150    134
   1   -62     30      6   117   -134     -8   -62    -26      1   -63     96
   2   132   -111     -8   -64     57     -7   127    108     -5   178   -173
   3   -64     16     -7   242    247     -6   349    353     -4   -65     67
  -7   -65    -41     -6   177   -167     -5   -58    -42     -3   -62     20
  -6   -63     -8     -5   -60     47     -4   414    419     -2   -61    -65
  -5   -63    -73     -4   327    324     -3   155    156     -1   -61     58
  -4   301   -302     -3   176    163     -2   -63     71
  -3   -60     66     -2   -55    -54     -1   -99   -155   H=     0, K=   24
  -2   108     93     -1   344   -326
  -1   123   -133                       H=     2, K=   23      0   -55    -54
                    H=     4, K=   22                          1   -68    -53
H=     7, K=   21                          0   -54    -39      2   360    308
                       0   400   -399      1   -53     10      3   269   -294
   0   -64    -54      1   -59    -16      2   -56     52      4   -65     40
  -4   -65    -20      2   215   -213      3   278   -296      5   454   -444
  -3   205   -200      3    87    -81      4    95    126      6   -61      3
  -2   -63     11      4   -63     98      5   253   -263      7   221   -225
  -1   -62    -55      5   -62   -101      6   116   -120      8   -65    -59
                      -8   -65     -6      7   179   -181
H=     0, K=   22     -7   -62     25     -8   127    -90   H=     1, K=   24
                      -6   -63     83     -7   141    161
   0   -55    -45     -5   318    309     -6   -59     16      0  -100   -450
   1   243   -252     -4   529   -506     -5   163    151      1   -61     97
   2   357    416     -3   -59    113     -4   145   -145      2   -58     96
   3   241    308     -2   -55     35     -3    83     88      3   372    395
   4   -58     37     -1    82    -94     -2   155    124      4   534   -541
   5   -57     -8                         -1   194   -160      5   126   -169
   6   -60    -13   H=     5, K=   22                          6   -61    -76
   7   -61     48                       H=     3, K=   23      7   -62    -62
   8   116    -81      0   339   -328                         -8   244    242
                       1   128    138      0   531   -536     -7   -64     99
H=     1, K=   22      2   -58     20      1   169    169     -6   133    136
                       3   -60     -5      2   221   -194     -5   118   -114
   0   -58    128      4   166   -154      3   202    210     -4   -64     65
   1   -55    -44     -7   359   -341      4   312   -316     -3   221    237
   2   168    160     -6   117    118      5   114    109     -2   -59    -93
   3   -58    -65     -5   -63    -54      6   119   -127     -1   -71    200
   4   257   -270     -4   -60     12     -8   263    253
   L     FO      FC

H=      2,  K=    24

   0   221     210
   1   215    -219
   2   167    -161
   3   -59    -118
   4   -58      41
   5   -61     -32
   6   -61      64
  -8   118     113
  -7   -61       1
  -6    93     -60
  -5   133    -126
  -4   343     332
  -3   350    -356
  -2   145    -145
  -1    84     -63

H=      3,  K=    24

   0   172    -177
   1   273    -274
   2   -59     -74
   3   205     203
   4   192     205
   5   115    -128
   6   278     253
  -8   -66      32
  -7   106      83
  -6   357    -365
  -5   -58     -30
  -4   230    -202
  -3   -57      18
  -2   278    -303
  -1   125    -128

H=      4,  K=    24

   0   -60     -98
   1   -62      47
   2   213    -212
   3   405     392
   4   -62     -41
  -7   200    -199
  -6    93     123
  -5   216    -202
  -4   170    -182
  -3   199    -200
  -2   166    -156
  -1   -61      99

H=      5,  K=    24

   0   202     199
   1   177    -154
   2   155     147
   3    94     -94
  -6   -65      71
  -5   136    -108
  -4   -62     -43
  -3   256    -254
  -2   261     264
  -1   -63     -57

H=      6,  K=    24

   0   -63     -30
  -5   137     132
  -4   -63     -43
  -3   126     123
  -2   -63     -28
  -1   220     228

H=      0,  K=    25

   1   189    -215
   2   -83      17
   3   -73      -3
   4   350    -376
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```
   L     FO      FC

   5   -62     -83
   6   168    -159
   7   -62     -24

H=      1,  K=    25

   0  -110    -255
   1   349    -368
   2   -62      70
   3   360    -456
   4   -73     208
   5   340    -330
   6   -61     -50
   7   -65     -53
  -7   230     229
  -6   -62      47
  -5   -60     -86
  -4   366    -378
  -3   -74    -116
  -2   -63     101
  -1   -76    -137

H=      2,  K=    25

   0   253    -240
   1    98      90
   2   525    -525
   3   -57      29
   4   113     101
   5   231     228
   6   -61     -19
  -7   -63     -92
  -6   -59     -37
  -5   137    -125
  -4   300    -295
  -3   -59    -119
  -2   495    -497
  -1   -54      20

H=      3,  K=    25

   0   -57      28
   1   -58      16
   2   -59       7
   3   -61     -15
   4   168     183
   5   214     224
  -7   145    -135
  -6   -61     -27
  -5   238    -249
  -4   169    -182
  -3   387    -374
  -2   313     308
  -1   244    -266

H=      4,  K=    25

   0   -60       3
   1   -59      22
   2   203     197
   3   -63     -26
   4   -63      53
  -7   -66     -66
  -6   115     -95
  -5   167     162
  -4   196    -177
  -3   -62      86
  -2   -61     -19
  -1   210     199

H=      5,  K=    25

   0   -62      38
   1   -63      57
   2   111    -113
  -6   138     128
  -5   -63     -61
  -4   -61       9
  -3   -61     -32
  -2    94     112
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```
   L     FO      FC

  -1   312     322

H=      6,  K=    25

  -3   158     137
  -2   147     161
  -1   148    -140

H=      0,  K=    26

   0   460    -479
   1   -80     130
   2   398    -398
   3   233    -289
   4   267    -278
   5   -60      42
   6   -62     -18
   7   -63     -84

H=      1,  K=    26

   0   -79     -18
   1   -94     -71
   2   260    -263
   3   -94     -91
   4   -65     108
   5   -63      75
   6   185    -177
  -7   -65     -26
  -6   246     251
  -5   376    -386
  -4   -77    -229
  -3   340    -356
  -2   124     177
  -1   281    -340

H=      2,  K=    26

   0   103     122
   1   101    -104
   2   -63    -108
   3   -62    -122
   4   235     245
   5   -61      19
   6   190     175
  -7   -64      -6
  -6   163    -147
  -5   -63     -23
  -4   202    -194
  -3   179    -169
  -2   -61     -67
  -1   -56      37

H=      3,  K=    26

   0   122     122
   1    96      95
   2   157    -181
   3   464     454
   4   127      99
   5   136     122
  -7   134    -127
  -6   -63     -89
  -5   -62     -63
  -4   -60      50
  -3   155     164
  -2   242    -257
  -1   237     241

H=      4,  K=    26

   0   333     320
   1   -61      38
   2   218     222
   3   109     140
  -6   165     174
  -5   171    -155
  -4   236     238
  -3   116     119
  -2   403     373
```

```
   L     FO      FC

  -1   155    -172

H=      5,  K=    26

   0   123     126
   1   -64      89
  -5   104     132
  -4   -64     -30
  -3   248     236
  -2   -63       3
  -1    99     107

H=      0,  K=    27

   1   300    -358
   2   -68      76
   3   175    -226
   4   -61      66
   5   -62     -73
   6   238     230

H=      1,  K=    27

   0   -58    -109
   1   -61     -31
   2   -81     -41
   3   237     257
   4   -62      25
   5   -61     -37
   6   196     199
  -6   -64     -70
  -5   104    -134
  -4   243    -273
  -3   -85      68
  -2   422    -447
  -1   -88     273

H=      2,  K=    27

   0   205     208
   1   112     101
   2   -59      30
   3   363     351
   4   147     156
   5   123     108
  -6   -62     -19
  -5   221    -236
  -4   -62      52
  -3   -57     -34
  -2   145     134
  -1   -59     -46

H=      3,  K=    27

   0   239     244
   1    95      95
   2   289     267
   3   -66      59
   4   198     180
  -6   -61      15
  -5   233     227
  -4    95      87
  -3   147     156
  -2   -63     109
  -1   197     185

H=      4,  K=    27

   0   197    -201
   1   245     241
   2   161     157
   3   -63      59
  -5   -65      18
  -4   174     163
  -3   245     228
  -2    94      99
  -1   240     232
```

```
   L     FO      FC      L     FO      FC      L     FO      FC      L     FO      FC

                                                 -5    -63      46     -4    101      63
H=     5, K=     27      0    -63     112     -4    -62     -19     -3     92     -86
                         1    -62      36     -3    -60      41     -2    126     120
   0    111     109      2    118     113     -2    138     135     -1    121     124
  -4    128     142      3    -65     -58     -1    -76      68
  -3    177    -190     -5    216     213                         H=     3, K=     30
  -2    169     162     -4    235     250   H=     3, K=     29
  -1    107      75     -3    -62     -13                            0    195    -157
                        -2    238     222      0    -61       3      1    256    -243
H=     0, K=     28     -1    -62      37      1    147     136     -3    120     -85
                                               2    264    -249     -2    -63      41
   0    -60      17   H=     4, K=     28     -4    -64      84     -1    154    -138
   1    145     176                           -3    155     157
   2    121     104      0    -62       0     -2    169    -186   H=     0, K=     31
   3     98     124      1    -65     -36     -1    -61      54
   4    -67     -62      2    -62     -35                            1    151     167
   5    249     239     -4    -63      -5   H=     4, K=     29      2    117    -111
   6    -65     -53     -3    109      84                            3    -66     -29
                        -2    -63     -17      0    -62     -26
H=     1, K=     28     -1    -65     -55     -3    -64     -74   H=     1, K=     31
                                              -2    -65      45
   0    135     185   H=     0, K=     29     -1    226    -228      0    -62      37
   1    -61     113                                                  1    -74     -73
   2    312     315      1    174     178   H=     0, K=     30      2    105     100
   3    -80     -82      2    110     107                            3    -65    -121
   4    211     223      3    -62      87      0    573     556     -3    -78     -42
   5    115      87      4    187     216      1    -67     -62     -2    -67     119
  -6    102    -131      5    -64      31      2    -64      34     -1    114    -135
  -5    -64       0                            3    -62      63
  -4    -75    -118   H=     1, K=     29      4    100     119   H=     2, K=     31
  -3    -61      32
  -2    -96     171      0    -73     176   H=     1, K=     30      0    123    -123
  -1    -79    -169      1    162     201                            1    135     -97
                         2    -63     124      0    -71      -5      2    -66     -52
H=     2, K=     28      3    213     202      1    -77     203     -3    -64      43
                         4    -74    -101      2    -66      10     -2    -68     -76
   0    -65    -129     -5    -64     -30      3    -73     -48     -1    -71      31
   1    141     141     -4    -66     106      4    -66      -5
   2    183     177     -3    -70      -9     -4    -68      46   H=     0, K=     32
   3    178     182     -2    -71       7     -3    235     249
   4    116     112     -1    -71      94     -2    -67    -116      0    115     130
  -6    -63      19                           -1    -70     134      1    -69     -44
  -5     92     104   H=     2, K=     29                            2    157    -156
  -4    208    -186                         H=     2, K=     30
  -3    -60      50      0    281     262                         H=     1, K=     32
  -2    119      83      1    112    -114      0    -80     -26
  -1    440     448      2    -64     -24      1    -65     -48      0    -63     -35
                         3    -63      59      2    124    -114      1    -63     -11
H=     3, K=     28      4    -65      93      3    -63     -47     -2    -77     -34
```

```
  L    FO     FC

H=    0,  K=    0

  2   249    193
  4  1324   1293
  6   526    526
  8   390   -399
 10   -55    -38

H=    1,  K=    0

  1   285    267
  3    83     92
  5   242   -285
  7   126    102
  9   701   -715
-11   -56     -2
 -9   384    412
 -7   832    820
 -5   786    833
 -3  1839   1825
 -1  1955   1890

H=    2,  K=    0

  0   859   -801
  2   354    357
  4   494   -469
  6   206   -180
  8   625   -610
-10   541    536
 -8   260    253
 -6   338    336
 -4    77     74
 -2  1049  -1028

H=    3,  K=    0

  1  1522  -1554
  3   996  -1007
  5   689   -704
  7   -57   -116
  9   153    130
-11   464    467
 -9   196   -179
 -7   302    269
 -5   145   -120
 -3   677   -652
 -1  1272  -1310

H=    4,  K=    0

  0  1284  -1276
  2   710   -737
  4   309   -327
  6   508    509
  8   -59     35
-10   122   -116
 -8   325    316
 -6  1171  -1150
 -4   234   -223
 -2  1683  -1676

H=    5,  K=    0

  1   332   -340
  3   577    605
  5   246   -239
  7   263    265
 -9   116   -114
 -7   530   -519
 -5   574   -570
 -3   153   -120
 -1   177   -140

H=    6,  K=    0

  0   141    131
  2   245    258
  4   -60     86
```

```
  L    FO     FC

 -8   355   -350
 -6   -59   -103
 -4   -51     -9
 -2   -51     34

H=    7,  K=    0

  1   429    433
  3   219    202
 -7   141   -167
 -5   308    300
 -3    84     53
 -1   443    421

H=    8,  K=    0

  0   140    137
 -6   -63     23
 -4   378    400
 -2   360    347

H=    0,  K=    1

  1  1128   1156
  2   158    157
  3    79    -93
  4   908   -907
  5   770    797
  6   379   -373
  7   302   -294
  8   459   -431
  9   106    -63
 10   305   -303

H=    1,  K=    1

  0   911    909
  1   979  -1013
  2   674    680
  3   486   -512
  4   294   -293
  5   347   -363
  6   -45    -51
  7   263   -282
  8   668   -657
  9   -56     29
 10   247   -248
-11   356    349
-10   110     74
 -9   329    320
 -8   345    343
 -7   257    260
 -6   182    191
 -5   -40     29
 -4   537    544
 -3   313   -318
 -2    64     66
 -1   764   -742

H=    2,  K=    1

  0  2436  -2452
  1   362   -373
  2   307    279
  3    58     34
  4   563   -574
  5   396   -443
  6   -47    -13
  7   198   -196
  8   117    121
  9   138   -133
-11   141    146
-10   -55     23
 -9   220    220
 -8   449    446
 -7   449    457
 -6   800   -787
 -5   567    579
 -4   -40    -83
 -3   229    185
```

```
  L    FO     FC

 -2   122    100
 -1   258   -249

H=    3,  K=    1

  0   437   -442
  1  1012  -1053
  2   783   -794
  3   245    273
  4   235   -241
  5    70    -44
  6   209   -197
  7   237    230
  8    87    -24
  9   329    326
-11   -60     51
-10   337    328
 -9   174   -160
 -8   222    227
 -7   536   -601
 -6   500    484
 -5   603   -613
 -4   489   -480
 -3   692   -717
 -2   643   -638
 -1   957   -962

H=    4,  K=    1

  0   154    129
  1    62     20
  2   288    306
  3   737   -790
  4   338    337
  5   -51    -18
  6   261    254
  7   221    227
  8   165    178
-10   417   -419
 -9   269    262
 -8   480   -487
 -7   591   -584
 -6   570   -580
 -5   428   -420
 -4   201   -193
 -3   230   -215
 -2   211   -204
 -1   945   -924

H=    5,  K=    1

  0   335   -355
  1   363    352
  2   142    121
  3   183    189
  4   -58     32
  5   243    236
  6   222    214
  7   -61    -35
-10   268   -276
 -9    83    -53
 -8   219   -224
 -7   282   -275
 -6   321   -317
 -5   366    355
 -4   367   -370
 -3   -46     44
 -2   114    113
 -1   473    461

H=    6,  K=    1

  0   187    187
  1   260    252
  2   362    400
  3   265    249
  4   -58    -20
  5   123    116
 -9   111   -116
 -8   102     97
```

```
  L    FO     FC

 -7   209   -222
 -6   185    197
 -5   -52    -13
 -4   255    243
 -3   -51    -38
 -2   444    446
 -1   129    103

H=    7,  K=    1

  0   326    337
  1   -63     87
  2   178    213
  3   165   -158
 -8   158   -144
 -7   278    287
 -6   153    136
 -5   460    473
 -4   174    211
 -3    91     91
 -2   126    136
 -1   261    275

H=    8,  K=    1

  0   182   -180
 -6   131    122
 -5   123    113
 -4   104    -63
 -3   328    300
 -2   -64     49
 -1   -62    -20

H=    0,  K=    2

  0    67     -4
  1   536   -517
  2   194   -189
  3   753   -759
  4   320   -360
  5   943   -940
  6   227   -200
  7   763   -751
  8   137    147
  9   750   -743
 10   116    102

H=    1,  K=    2

  0  1568  -1550
  1   573   -555
  2  1476  -1426
  3    92    -63
  4   700   -654
  5   239   -215
  6   755   -742
  7   -48     -9
  8   213   -191
  9   130   -124
 10   -57     -8
-11   -58    -75
-10   639    632
 -9   456    438
 -8    84     85
 -7   335   -341
 -6   381    385
 -5   126   -119
 -4   232   -197
 -3   322    304
 -2   463   -455
 -1   539   -512

H=    2,  K=    2

  0  1058  -1118
  1   402    356
  2    93    -84
  3   657   -662
  4   -41    -76
  5   253   -273
```

```
   L    FO     FC

   6   192   -192
   7   478    478
   8   -56    -41
   9    84    -47
 -11   -58    -15
 -10   -56    -50
  -9   -55    -33
  -8   273   -262
  -7   -47     92
  -6   399    395
  -5   868   -851
  -4   225   -219
  -3   662    629
  -2   258   -234
  -1  2839  -2801

H=     3,  K=     2

   0   129     91
   1   364    379
   2   246   -267
   3   377   -350
   4   722    713
   5   242    277
   6   117     94
   7   -57    -37
   8   623    607
   9   -60     42
 -11   170   -159
 -10   239   -241
  -9   109   -115
  -8   370   -350
  -7   206   -205
  -6   516   -533
  -5   568    549
  -4   964   -971
  -3   289   -281
  -2   674   -684
  -1   322   -347

H=     4,  K=     2

   0   851    881
   1   617    635
   2   -44     21
   3   826    828
   4   -50     58
   5   400    413
   6   197    184
   7   534    508
   8   -60    -59
 -10   151   -147
  -9   303   -301
  -8    75    -72
  -7   632   -648
  -6   -48    -21
  -5   405   -425
  -4   279    293
  -3   171    166
  -2   186   -180
  -1   354    357

H=     5,  K=     2

   0   659    650
   1   419    445
   2   492    498
   3   115     91
   4   244    237
   5   -57    -76
   6   135    136
 -10   -60      5
  -9   -57     32
  -8   311   -314
  -7   123    120
  -6   -51    -31
  -5    77     69
  -4   511    522
  -3   345    339
  -2   -46     35
```

```
   L    FO     FC

  -1   176    176

H=     6,  K=     2

   0   -52     81
   1   102    120
   2   117    112
   3   268    277
   4    97     94
   5   260   -260
  -9   265   -255
  -8   104    101
  -7   436    448
  -6   275    273
  -5   106    -79
  -4   273   -273
  -3   457    462
  -2   246    253
  -1   291    290

H=     7,  K=     2

   0   129    132
   1   -62     93
   2   262   -258
   3   124   -110
  -8   222    222
  -7   -63     37
  -6   264    251
  -5    88    -78
  -4   374    367
  -3   -59     67
  -2   152    146
  -1   166   -162

H=     8,  K=     2

   0   189   -177
  -6   -62    -18
  -5   102    106
  -4   113   -112
  -3   -62    -17
  -2   -61     -3
  -1   152   -139

H=     0,  K=     3

   1   872   -869
   2   789   -807
   3   771   -817
   4   702   -718
   5   687   -692
   6   922   -924
   7   283    268
   8    91   -108
   9   118     82
  10   164   -156

H=     1,  K=     3

   0   397   -376
   1   775    791
   2   501   -516
   3   656   -665
   4   269    276
   5    60     77
   6   384    379
   7   124    -86
   8    85    -19
   9   129   -138
  10   333    319
 -11   -57     74
 -10   -55    -38
  -9   520    499
  -8    75    -51
  -7   162    176
  -6   584   -580
  -5   922    898
  -4   324   -296
  -3   706   -657
```

```
   L    FO     FC

  -2   722   -700
  -1   640   -635

H=     2,  K=     3

   0   823    799
   1   309    342
   2   471    449
   3   907    910
   4   542   -544
   5   116    -94
   6   192    183
   7   304    307
   8   -56     70
   9   192    196
 -11    99    -98
 -10   -54    -28
  -9   283   -292
  -8   192    175
  -7   159   -144
  -6   407   -421
  -5   291   -286
  -4   266    255
  -3   173    155
  -2   178    164
  -1  1393  -1326

H=     3,  K=     3

   0  1742   1744
   1   121   -128
   2   477    465
   3   232    226
   4   382    389
   5   121     99
   6   439    464
   7   547    539
   8    91     65
   9   252    249
 -11   -60     49
 -10   252   -244
  -9   359   -380
  -8   540   -531
  -7    87    -72
  -6    98   -121
  -5   505   -507
  -4   355    348
  -3   169   -197
  -2   397   -377
  -1   299   -366

H=     4,  K=     3

   0   528    542
   1   375    407
   2   361    369
   3   459    458
   4   558    573
   5    74     14
   6   217    235
   7   -59     76
   8   165    152
 -10   178   -169
  -9   203   -197
  -8   283   -281
  -7   246    230
  -6   519   -524
  -5   315    343
  -4   386   -403
  -3   896    901
  -2   168   -149
  -1  1194   1241

H=     5,  K=     3

   0    79     38
   1   258    257
   2   118    129
   3   193    190
   4   166   -178
```

```
   L    FO     FC

   5    82     64
   6   100    -93
 -10   208    192
  -9   -59     15
  -8   295    300
  -7   114   -100
  -6   -51    -16
  -5    94    -40
  -4   476    470
  -3   415    434
  -2   342    349
  -1    89     97

H=     6,  K=     3

   0   375   -393
   1   415   -438
   2   253    244
   3   -60    -93
   4   -59     36
   5   252   -267
  -9   -59     14
  -8   270    243
  -7   254    256
  -6   189    191
  -5    92    108
  -4    82     -5
  -3    86    -87
  -2   429    446
  -1   -52     31

H=     7,  K=     3

   0   460   -479
   1   201   -215
   2   323   -315
   3    91    -86
  -8   398    397
  -7   172    160
  -6   161   -154
  -5   217    235
  -4   178   -182
  -3   -59    -31
  -2   436   -442
  -1   176    183

H=     8,  K=     3

   0    97    -86
  -6   -64    -50
  -5   235   -240
  -4   100    121
  -3   358   -369
  -2   126   -132
  -1   156   -141

H=     0,  K=     4

   0  1284  -1258
   1   111   -118
   2   769   -761
   3   987    971
   4  1322  -1342
   5   292   -283
   6   138   -117
   7   240    268
   8   187    183
   9   -53     15
  10   122    111

H=     1,  K=     4

   0   103    111
   1   454    444
   2    60    -91
   3   389   -370
   4   719   -722
   5   705    679
   6   413    416
   7   181    173
```

```
    L    FO     FC

    8   413   -431
    9   416    433
   10   230    200
  -10   110    -82
   -9   -55      0
   -8   363   -357
   -7   655   -627
   -6   277   -263
   -5   860   -853
   -4   593    565
   -3   743   -735
   -2   478   -454
   -1   688   -675

 H=     2,  K=    4

    0   -40      5
    1    88    -53
    2   376    380
    3   -40     -9
    4   734    736
    5   138    117
    6   459    465
    7    77     93
    8   347    347
    9   -57    -23
  -11   -59    -70
  -10   294   -286
   -9   214   -216
   -8   222   -227
   -7   -47    -71
   -6   296   -290
   -5   113   -113
   -4   433   -424
   -3    99    108
   -2   345    360
   -1  1527  -1509

 H=     3,  K=    4

    0   -40    -14
    1   781    769
    2   641    666
    3   714    744
    4   -45    -31
    5   623    641
    6   259   -261
    7   181    176-
    8    86     94
  -11   439   -412
  -10   182   -191
   -9    81    -47
   -8   163    154
   -7   245   -252
   -6   236   -210
   -5   166   -123
   -4   156   -138
   -3   833    806
   -2   565    592
   -1   240    249

 H=     4,  K=    4

    0   224    194
    1   457   -469
    2   348    330
    3   128   -145
    4   289    317
    5   -53     44
    6   268   -264
    7   205   -216
    8   -61    -80
  -10   -58     -6
   -9   276    289
   -8   -52    -37
   -7   -50    -36
   -6   588    568
   -5   562    543
   -4   241    219
   -3   415   -405

    L    FO     FC

   -2  1357   1373
   -1   837    826

 H=     5,  K=    4

    0   593   -624
    1   -48    -21
    2   290    273
    3   244   -244
    4   108   -151
    5   202   -216
    6   -59    -59
  -10   -60     48
   -9   193    195
   -8   524    524
   -7   257    245
   -6   221   -219
   -5   249    253
   -4   115   -122
   -3   465    446
   -2   301    317
   -1   -47      8

 H=     6,  K=    4

    0   118   -104
    1   149   -162
    2   380   -399
    3   120   -111
    4   120   -117
    5    95   -104
   -9   -61     25
   -8   153    153
   -7   -60    116
   -6   250    256
   -5   135   -134
   -4   -52    -38
   -3   -51      4
   -2   -52     13
   -1   160   -174

 H=     7,  K=    4

    0   128    -99
    1   316   -325
    2   174   -176
    3   256   -262
   -8   -65    -69
   -7   -62     15
   -6   -60     58
   -5   145   -158
   -4   233   -251
   -3   182   -171
   -2   -60     10
   -1   465   -478

 H=     8,  K=    4

    0   116   -123
   -6   131   -140
   -5   123    157
   -4   312   -307
   -3   -64    -19
   -2   375   -390
   -1   -64     15

 H=     0,  K=    5

    1   305   -320
    2    88     94
    3   375   -375
    4  1427 . 1435
    5   421   -410
    6   345    341
    7    77     59
    8   372    363
    9   -54     74
   10   203    174

 H=     1,  K=    5

    L    FO     FC


    0   694   -649
    1  1205   1166
    2   331   -297
    3   165    155
    4   483    463
    5   684    690
    6   -46      8
    7   199    188
    8   -56     41
    9   -55    -32
   10   -59     42
  -10   101     87
   -9   111     97
   -8   159   -169
   -7   573   -573
   -6   188   -184
   -5   232   -204
   -4   942   -950
   -3   470    458
   -2   321    296
   -1   850   -803

 H=     2,  K=    5

    0   338   -334
    1   149   -175
    2   274    262
    3   264    275
    4   -44     95
    5   422    398
    6   -48     -8
    7   200   -206
    8   -55     75
    9   175    190
  -11   142   -132
  -10   105   -112
   -9   -55     66
   -8   145   -133
   -7   327   -323
   -6   122    133
   -5   290   -261
   -4   214    231
   -3   311   -305
   -2   623    612
   -1   681   -669

 H=     3,  K=    5

    0   148   -151
    1   154   -125
    2   363    375
    3   125    152
    4   315    340
    5   542   -527
    6   -51      9
    7   -56    -21
    8   296    290
  -10   351  . -319
   -9   -56    -24
   -8   182    183
   -7   609    605
   -6   163   -169
   -5   143    139
   -4   397   -405
   -3   916    878
   -2   610    630
   -1   780    757

 H=     4,  K=    5

    0   -43    -51
    1   -44      0
    2   881   -876
    3   220    218
    4   245   -236
    5   -52     41
    6   610   -605
    7   -59     36
  -10   488    466

    L    FC     FC

   -9   131    110
   -8   111    108
   -7   235    243
   -6   576    551
   -5   172    150
   -4   326    349
   -3   631    631
   -2   327    322
   -1   720    724

 H=     5,  K=    5

    0   177    195
    1   139   -146
    2   220   -241
    3   332   -313
    4   -59     59
    5   263   -275
    6   201   -174
  -10   149    145
   -9   107    122
   -8   131    136
   -7   140    147
   -6   450    447
   -5   -50      0
   -4   221    204
   -3   -48     10
   -2   481    469
   -1   877   -900

 H=     6,  K=    5

    0   151   -144
    1   174    185
    2   110   -112
    3   258   -286
    4    93     45
    5    98    -95
   -9   -63    114
   -8   -60    -70
   -7   102    127
   -6   -58    -72
   -5   -54     89
   -4   371   -371
   -3   288    283
   -2   531   -547
   -1   299   -306

 H=     7,  K=    5

    0   -61    -26
    1   -62    -37
    2   205   -183
    3   230    207
   -8   142   -105
   -7   137   -138
   -6    91     97
   -5   363   -353
   -4   178   -136
   -3   338   -338
   -2   220   -222
   -1   -62     37

 H=     8,  K=    5

    0   314    323
   -5   108    -88
   -4   138    128
   -3   261   -268
   -2   -63      0
   -1   -63     -7

 H=     0,  K=    6

    0   190   -157
    1   434   -414
    2   251    260
    3  1017   1025
    4   231   -210
    5   787    748
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L	FO	FC
6	131	144
7	631	622
8	186	-171
9	385	331
10	87	-62
H=	1, K=	6
0	110	-35
1	885	-860
2	389	412
3	896	850
4	949	952
5	395	-385
6	721	710
7	268	-277
8	-56	-7
9	-55	30
10	-58	-57
-10	421	-399
-9	239	-249
-8	-49	8
-7	372	367
-6	266	-266
-5	642	-601
-4	-40	30
-3	235	233
-2	217	190
-1	560	544
H=	2, K=	6
0	651	602
1	59	21
2	320	-316
3	378	395
4	178	150
5	116	121
6	81	-86
7	-51	-31
8	85	-90
9	160	-152
-10	-57	86
-9	79	55
-8	-50	-2
-7	80	72
-6	151	-145
-5	234	218
-4	1145	1118
-3	601	582
-2	907	-813
-1	-40	47
H=	3, K=	6
0	-40	31
1	461	-488
2	138	144
3	407	414
4	324	-313
5	455	-465
6	428	-426
7	194	194
8	177	-144
-10	185	-180
-9	-55	-38
-8	380	375
-7	472	450
-6	718	711
-5	106	71
-4	739	723
-3	98	-103
-2	1275	1275
-1	-41	-36
H=	4, K=	6
0	217	-223
1	-44	60
2	155	-158

L	FO	FC
3	727	-738
4	82	-52
5	375	-347
6	-57	-19
7	335	-369
-10	-58	20
-9	431	422
-8	-57	36
-7	461	462
-6	-50	-71
-5	810	792
-4	303	-310
-3	100	-68
-2	-44	-20
-1	189	232
H=	5, K=	6
0	133	-113
1	-50	-56
2	179	-169
3	-52	12
4	358	-373
5	147	140
6	106	-98
-10	206	194
-9	138	-128
-8	-58	27
-7	154	-129
-6	-52	22
-5	-50	-19
-4	133	-117
-3	224	-240
-2	74	-18
-1	-48	0
H=	6, K=	6
0	166	164
1	197	-193
2	180	196
3	-59	-82
4	-61	-77
5	-62	41
-9	131	-134
-8	192	179
-7	107	-87
-6	340	-354
-5	100	-94
-4	192	174
-3	373	-384
-2	220	-222
-1	360	-381
H=	7, K=	6
0	-62	-85
1	-62	-57
2	-64	54
3	211	190
-8	409	-401
-7	135	114
-6	322	-331
-5	-62	-22
-4	530	-558
-3	-61	15
-2	335	-346
-1	376	400
H=	8, K=	6
0	105	79
-5	123	-107
-4	114	98
-3	-65	-56
-2	141	135
-1	-66	109
H=	0, K=	7

L	FO	FC
1	1509	1455
2	786	782
3	1495	1467
4	278	271
5	-42	41
6	264	233
7	107	117
8	80	-98
9	-55	-68
10	217	198
H=	1, K=	7
0	-41	-75
1	203	-221
2	97	-94
3	365	327
4	254	246
5	236	248
6	497	-510
7	-50	-30
8	121	109
9	276	282
10	238	-231
-10	-56	-7
-9	179	-178
-8	226	229
-7	107	-128
-6	950	921
-5	132	117
-4	635	615
-3	803	-763
-2	1232	1195
-1	378	347
H=	2, K=	7
0	296	-261
1	652	659
2	336	338
3	491	-506
4	65	56
5	-45	-20
6	110	101
7	491	-475
8	234	244
9	183	-186
-10	345	-348
-9	339	319
-8	215	223
-7	-47	54
-6	182	-168
-5	650	664
-4	270	302
-3	123	-114
-2	267	304
-1	164	-137
H=	3, K=	7
0	997	-1007
1	304	301
2	489	-502
3	223	-226
4	926	-921
5	-50	-34
6	346	-352
7	-57	68
8	133	-139
-10	81	20
-9	130	141
-8	200	204
-7	-50	75
-6	181	183
-5	515	501
-4	157	-167
-3	-41	28
-2	63	52
-1	843	805

L	FO	FC
H=	4, K=	7
0	148	-142
1	786	-768
2	182	-165
3	257	-267
4	354	-352
5	-57	-57
6	-56	34
7	-59	33
-10	-60	82
-9	89	-89
-8	369	360
-7	284	-279
-6	135	143
-5	440	-433
-4	74	50
-3	1093	-1139
-2	851	822
-1	820	-835
H=	5, K=	7
0	135	142
1	168	-147
2	118	-103
3	313	-324
4	273	276
5	92	82
6	90	92
-10	-62	20
-9	164	149
-8	581	-569
-7	110	89
-6	240	-260
-5	163	168
-4	609	-611
-3	135	-141
-2	457	-441
-1	280	-266
H=	6, K=	7
0	153	-159
1	303	311
2	105	-95
3	147	149
4	-61	-31
5	297	297
-9	-62	1
-8	-60	21
-7	249	-253
-6	-60	8
-5	281	-282
-4	364	-379
-3	-53	65
-2	219	-239
-1	88	-95
H=	7, K=	7
0	174	184
1	95	-115
2	354	340
3	95	-73
-8	-66	-38
-7	171	-185
-6	-64	89
-5	-60	-5
-4	-62	-10
-3	381	-398
-2	518	527
-1	184	169
H=	8, K=	7
-5	299	304
-4	146	-125
-3	282	297
-2	185	186

```
   L    FO     FC

  -1   218    214

H=     0,  K=    8

   0   434    485
   1   308    770
   2  1350   1367
   3   910   -845
   4   254    222
   5    95   -104
   6   147    151
   7   364   -347
   8   274    272
   9   260   -263
  10   393   -380

H=     1,  K=    8

   0   406   -380
   1   116   -105
   2   868   -879
   3   -40     13
   4   348    330
   5    80    -78
   6   399   -409
   7   404   -397
   8   -56    -24
   9   305   -279
 -10   -58     46
  -9   166    179
  -8   -50    -31
  -7   425    430
  -6   524    520
  -5   507    513
  -4   211   -214
  -3   712    721
  -2   239    242
  -1  1058   1009

H=     2,  K=    8

   0   212    188
   1   -40    -14
   2   611   -613
   3   197   -184
   4   335   -341
   5    83    -60
   6   277   -280
   7   164    174
   8   390   -397
   9   -60    -58
 -10   234    245
  -9   133   -117
  -8   445    435
  -7   -48    -69
  -6   258    271
  -5   171    191
  -4   774    722
  -3   299   -292
  -2   174   -207
  -1   577   -582

H=     3,  K=    8

   0   261    245
   1   452   -467
   2   351   -353
   3   655   -666
   4   229    216
   5   531   -520
   6   112    119
   7   -55    -60
   8   175    156
 -10   -57     27
  -9   331    323
  -8   418   -411
  -7   338    318
  -6    86   -108
  -5    65    -85
  -4   789   -786
```

```
   L    FO     FC

  -3    77    -46
  -2   453   -435
  -1   394   -382

H=     4,  K=    8

   0   618   -624
   1   323    343
   2   708   -721
   3   265    275
   4   123   -128
   5   112    103
   6   -57    -21
   7   299    309
 -10   116    128
  -9   137   -170
  -8   204   -195
  -7   108   -116
  -6   -50     38
  -5   779   -788
  -4   893   -862
  -3   113    110
  -2   227   -218
  -1   -44      0

H=     5,  K=    8

   0   307    314
   1   208   -204
   2   -53    -88
   3   -54    -21
   4   316    327
   5   325    346
   6   -63    -93
  -9   131   -133
  -8   -58    -17
  -7   489   -471
  -6   -52    -11
  -5   189   -185
  -4   -50      7
  -3   716   -739
  -2   -50     85
  -1   130   -111

H=     6,  K=    8

   0   -53     18
   1   -57     23
   2   309    318
   3   -60      0
   4   112    100
   5   -63    -44
  -9   -61     -6
  -8   272   -273
  -7   271    286
  -6   389   -397
  -5   118    114
  -4    87    -55
  -3   159    178
  -2   167   -171
  -1   150    122

H=     7,  K=    8

   0   101    109
   1   326    314
   2   242   -227
   3   326    321
  -7   -64    -86
  -6   167    161
  -5    98    101
  -4   308    292
  -3   150    150
  -2   -62     16
  -1   251    241

H=     8,  K=    8

  -5   -65     44
  -4   253    254
```

```
   L    FC     FC

  -3   -63     43
  -2   276    283
  -1   -64    -10

H=     0,  K=    9

   1    70     76
   2   487   -499
   3   240    270
   4   955   -959
   5   298   -304
   6   660   -674
   7   394    404
   8   883   -951
   9   268   -253
  10   205   -220

H=     1,  K=    9

   0   982    945
   1   892   -875
   2   241   -200
   3   909   -889
   4   361    347
   5   658   -609
   6    73    -51
   7   292   -284
   8   -55      9
   9   337   -308
 -10   202    198
  -9   276    291
  -8   199   -196
  -7   548    552
  -6   135    152
  -5   -42    -19
  -4   202   -179
  -3    72   -106
  -2   298   -299
  -1   430   -405

H=     2,  K=    9

   0   215   -207
   1   -40    -57
   2  1009  -1000
   3   133    124
   4    68     69
   5   251   -264
   6   126   -138
   7   224    236
   8   -57    -53
   9   194   -187
 -10   104    130
  -9   -55    -41
  -8   237   -238
  -7    72     -7
  -6   -45    -37
  -5   126    117
  -4   515   -491
  -3   108    114
  -2   261   -272
  -1   515    453

H=     3,  K=    9

   0   324   -312
   1   132   -140
   2   121   -127
   3    95    -94
   4   325   -309
   5   338    350
   6   164    174
   7   325    337
   8   284   -276
 -10   104    100
  -9   290   -304
  -8   349    357
  -7   716   -728
  -6   -48    -62
  -5   459   -463
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```
   L    FO     FC

  -4   349    404
  -3   992  -1008
  -2   374   -385
  -1   394   -389

H=     4,  K=    9

   0   125    134
   1   664   -650
   2   786    792
   3    93     81
   4   447    457
   5   171   -181
   6   525    515
   7   241   -229
 -10   460   -447
  -9   119   -108
  -8   437   -440
  -7   215    213
  -6   649   -675
  -5   310   -319
  -4   529   -514
  -3   327   -328
  -2   162    170
  -1   -44     22

H=     5,  K=    9

   0   134    145
   1   318    311
   2   286   -289
   3   559    551
   4   -59    -47
   5   264    260
   6   103     96
  -9   290   -279
  -8   -58    -45
  -7    99   -117
  -6   248   -230
  -5   179    182
  -4   362    373
  -3    83     54
  -2   568   -555
  -1   433    437

H=     6,  K=    9

   0   272    261
   1   -60     32
   2   273    283
   3   179    172
   4   105    100
  -9    91    -81
  -8   162    168
  -7   -62    -70
  -6   175    192
  -5    99     93
  -4   413    419
  -3   222   -237
  -2   -54     67
  -1   209    211

H=     7,  K=    9

   0   -62     11
   1   151    143
   2   334    340
  -7   267    255
  -6   -64    -74
  -5   391    388
  -4   116    128
  -3   287    288
  -2   299    319
  -1   -61     17

H=     8,  K=    9

  -4   -65     -7
  -3   -63      9
  -2    92     54
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L	FO	FC
-1	-65	49
H= 0, K= 10		
0	1295	-1261
1	156	144
2	470	-460
3	847	-804
4	595	-631
5	595	-619
6	74	-95
7	350	-332
8	-56	-4
9	538	-539
10	-57	3
H= 1, K= 10		
0	1276	-1229
1	99	-89
2	545	-518
3	-42	-24
4	166	-173
5	440	448
6	285	-286
7	109	107
8	117	-103
9	246	244
-10	298	281
-9	325	-241
-8	459	441
-7	539	-560
-6	161	147
-5	-42	-14
-4	103	117
-3	1115	-1065
-2	185	-181
-1	196	-207
H= 2, K= 10		
0	-40	32
1	853	-845
2	714	705
3	-43	-5
4	280	286
5	-48	-3
6	211	215
7	151	-163
8	334	343
9	366	358
-10	169	-171
-9	-55	-55
-8	394	-395
-7	183	-185
-6	-46	-61
-5	291	281
-4	605	-569
-3	495	-475
-2	186	-145
-1	181	-168
H= 3, K= 10		
0	121	-141
1	912	858
2	133	-124
3	372	370
4	-49	7
5	341	337
6	430	423
7	169	204
8	195	181
-10	190	-195
-9	123	-119
-8	-57	-59
-7	310	-299
-6	572	-575
-5	93	-90
-4	141	-168
-3	133	155
-2	770	-795
-1	358	347
H= 4, K= 10		
0	198	202
1	299	306
2	299	328
3	351	363
4	204	204
5	371	372
6	151	-150
7	178	174
-10	-60	-18
-9	409	-391
-8	-55	28
-7	340	-345
-6	436	460
-5	623	-661
-4	379	389
-3	-46	-92
-2	596	625
-1	228	225
H= 5, K= 10		
0	-50	46
1	262	262
2	441	437
3	326	-336
4	242	247
5	-59	-28
6	98	-94
-9	311	304
-8	183	-200
-7	130	129
-6	-54	-71
-5	354	359
-4	-51	13
-3	136	111
-2	409	406
-1	225	-211
H= 6, K= 10		
0	-60	-51
1	420	433
2	280	-294
3	-61	-66
4	191	-194
-8	-61	-8
-7	137	-126
-6	117	149
-5	510	523
-4	98	100
-3	102	-103
-2	-53	-45
-1	225	216
H= 7, K= 10		
0	-63	-32
1	194	-195
2	-66	70
-7	-64	39
-6	177	159
-5	-64	-86
-4	248	252
-3	-62	-84
-2	294	301
-1	287	-286
H= 8, K= 10		
-3	90	62
-2	140	-143
H= 0, K= 11		
1	1329	-1306
2	563	496
3	1073	-1073
4	410	363
5	262	-275
6	-48	-42
7	182	-171
8	226	236
9	267	253
10	92	-64
H= 1, K= 11		
0	855	-851
1	191	188
2	492	-466
3	360	355
4	283	269
5	353	-356
6	242	240
7	387	386
8	426	418
9	-60	-111
-10	151	-136
-9	-56	-65
-8	291	-283
-7	185	190
-6	660	-633
-5	266	-267
-4	702	-705
-3	353	365
-2	628	-643
-1	691	-673
H= 2, K= 11		
0	200	-160
1	128	168
2	658	-652
3	363	378
4	419	428
5	480	493
6	298	-314
7	256	244
8	255	222
9	242	235
-10	265	263
-9	479	-482
-8	144	-173
-7	348	-341
-6	403	375
-5	346	-351
-4	242	-254
-3	290	-306
-2	218	-210
-1	275	244
H= 3, K= 11		
0	603	607
1	458	481
2	937	941
3	595	-592
4	475	479
5	-52	-44
6	273	257
7	-58	91
8	133	127
-10	346	-344
-9	136	152
-8	348	-354
-7	126	-127
-6	-49	78
-5	142	-123
-4	-45	37
-3	471	462
-2	827	833
-1	666	-654
H= 4, K= 11		
0	113	90
1	938	930
2	277	-282
3	140	113
4	-52	50
5	143	147
6	-58	12
7	138	-138
-10	-60	20
-9	-58	-13
-8	96	99
-7	274	309
-6	139	-124
-5	593	593
-4	113	116
-3	574	569
-2	-47	7
-1	612	626
H= 5, K= 11		
0	202	209
1	-57	-63
2	-54	-36
3	346	331
4	152	-139
5	-60	-85
6	242	-258
-9	-62	-90
-8	236	242
-7	85	92
-6	375	365
-5	110	-104
-4	338	361
-3	131	138
-2	117	88
-1	299	294
H= 6, K= 11		
0	291	287
1	166	-178
2	-60	-54
3	195	-199
4	-61	4
-8	-63	-63
-7	110	103
-6	-59	85
-5	206	206
-4	249	265
-3	92	-86
-2	126	-143
-1	147	-124
H= 7, K= 11		
0	217	-227
1	-64	27
2	337	-332
-7	189	195
-6	-64	-20
-5	229	-236
-4	178	-174
-3	168	152
-2	351	-338
-1	113	-136
H= 0, K= 12		
0	1475	-1447
1	344	346
2	1293	-1319
3	570	561
4	113	-118
5	453	432
6	81	-62
7	353	346
8	-54	71
9	265	257

```
   L    FO    FC

H=    1,  K=   12

   0    80    84
   1   248  -225
   2   937   891
   3   -43     3
   4   268   269
   5   -47   -24
   6   369   365
   7   332   323
   8   191   183
   9   235   227
 -10   354  -343
  -9   215  -201
  -8    78   -37
  -7   -49   -21
  -6   -48   -67
  -5   663  -650
  -4   276  -307
  -3   271  -287
  -2   841   847
  -1   823  -838

H=    2,  K=   12

   0   452   451
   1   263   235
   2   -44    -6
   3   241   235
   4    88    82
   5   201   193
   6   268   243
   7   -56   -22
   8   177   174
 -10   184  -199
  -9   162  -154
  -8   114  -125
  -7   -50    30
  -6   197  -196
  -5   712   724
  -4    70   -60
  -3   -42    41
  -2   306   320
  -1   649   651

H=    3,  K=   12

   0   506   490
   1   261   282
   2   363   306
   3   429   440
   4   472  -442
   5   269   279
   6   -56   -49
   7   -59   -82
   8   242  -219
 -10   101   106
  -9   201  -183
  -8   324   348
  -7   -52    65
  -6   265   265
  -5   -49   -40
  -4   641   636
  -3   139   174
  -2   104   119
  -1  1081  1090

H=    4,  K=   12

   0   663   648
   1   123  -117
   2   336   340
   3   491  -507
   4   -57   -65
   5   492  -496
   6   -60   -60
   7   -60   -51
  -9   421   415
  -8   -57    54

   L    FO    FC

  -7   107   110
  -6   -51     3
  -5   224   253
  -4   723   717
  -3   259   272
  -2   376   385
  -1   139  -130

H=    5,  K=   12

   0   391  -407
   1    97  -108
   2   265  -290
   3   -58    13
   4   -58   -32
   5   171  -194
  -9   -62   -80
  -8   -59    55
  -7   358   356
  -6   -58    -2
  -5   219   193
  -4   186  -195
  -3   187   157
  -2   241  -246
  -1   130   128

H=    6,  K=   12

   0   107  -100
   1   -60   -19
   2   147  -152
   3   -61   -77
   4   -54   -76
  -8   154   139
  -7   294  -296
  -6   -60    28
  -5    90   -84
  -4   -60    76
  -3   313  -311
  -2   130  -150
  -1   191  -179

H=    7,  K=   12

   0   188  -198
   1   318  -320
  -6   283  -277
  -5   -64   -21
  -4   125  -110
  -3   219  -212
  -2   -65    52
  -1   120  -148

H=    0,  K=   13

   1   313   314
   2   422   427
   3   443  -414
   4   346   366
   5   367   384
   6   781   787
   7   153  -135
   8   291   289
   9   -57    81

H=    1,  K=   13

   0   629  -618
   1   163   188
   2   460   455
   3   913   899
   4   615  -586
   5   412   377
   6   191   185
   7   114    96
   8   151   161
   9   -59   -17
  -9   463  -466
  -8   137   170
  -7   110  -119

   L    FO    FC

  -6   111  -116
  -5   -46    17
  -4   -44    -1
  -3   155   146
  -2   364   421
  -1   900   884

H=    2,  K=   13

   0   403   393
   1   127   153
   2   601   574
   3   163  -141
   4   -47    -7
   5   -50    16
   6   -55   -59
   7   113   103
   8   247  -242
 -10    85   -96
  -9   -57    36
  -8   -55   -88
  -7   188  -196
  -6   158   138
  -5   -45    13
  -4   434   430
  -3   -44    59
  -2   529   540
  -1    74    86

H=    3,  K=   13

   0   152   144
   1   553   526
   2   175  -183
   3   487  -489
   4   316   297
   5   144  -129
   6   179  -190
   7   363  -365
  -9   179   217
  -8   189  -193
  -7   -53    61
  -6    86    76
  -5   833   858
  -4    89   -83
  -3   477   472
  -2   204   222
  -1   416   425

H=    4,  K=   13

   0   509  -496
   1   222   229
   2   240  -242
   3   -53   -63
   4   364  -373
   5   284   280
   6   315  -318
  -9   227   201
  -8   557   559
  -7   110  -112
  -6   122   124
  -5   -52    62
  -4   247   237
  -3   125   123
  -2   -48    28
  -1   270  -283

H=    5,  K=   13

   0   256  -262
   1   365  -385
   2   156   138
   3   -59   -37
   4    99    67
   5   186  -175
  -9   185   183
  -8   -59    41
  -7   217  -209
  -6    90   107

   L    FO    FC

  -5   -59    22
  -4   203  -210
  -3   366  -351
  -2   217   206
  -1   299  -310

H=    6,  K=   13

   0   319  -341
   1   150  -162
   2   -60    33
   3   -63   -97
  -8   -64   -54
  -7   113    83
  -6   -62   -56
  -5   135  -153
  -4   211  -226
  -3   -59    -3
  -2   342  -343
  -1   -59   -39

H=    7,  K=   13

   0   -64    26
   1   176   159
  -6   -65   -41
  -5   402  -397
  -4   -63   -29
  -3   154  -154
  -2   -64   -51
  -1   166  -182

H=    0,  K=   14

   0   578   610
   1   563   554
   2   713   676
   3   229   227
   4   665   651
   5   336   330
   6    74    46
   7   575   572
   8   226  -217
   9   181   174

H=    1,  K=   14

   0   731   676
   1   798   743
   2   233   215
   3    67   -92
   4   805   782
   5    86   -79
   6   160   167
   7   -55   -45
   8   209   212
   9   246  -239
  -9   -56    51
  -8   314  -310
  -7   150   128
  -6   -49   -40
  -5   395   361
  -4   -46   -60
  -3   701   656
  -2   -59   174
  -1   255  -262

H=    2,  K=   14

   0   149  -169
   1   275   310
   2   131   128
   3   209   232
   4   106   -92
   5   126   110
   6   365  -359
   7   206  -208
   8   -60    90
  -9   -57    81
  -8   224   222
  L     FO     FC

 -7    121   -125
 -6    -49    -49
 -5    220    217
 -4    109    -73
 -3    650    651
 -2    264    273
 -1    322    323

H=     3,  K=   14

  0    105    120
  1    609   -627
  2    246   -275
  3    382   -383
  4    -53    -42
  5    284   -263
  6    359   -373
  7    180   -182
 -9    257    263
 -8    -56      9
 -7    -56    -10
 -6    424    411
 -5    -51     69
 -4    403    396
 -3    478   -474
 -2    139    132
 -1    143   -147

H=     4,  K=   14

  0    514   -527
  1    238   -239
  2    252   -250
  3    364   -366
  4    164   -135
  5    316   -311
  6    163    152
 -9    147    140
 -8    106    114
 -7    312    326
 -6    405   -410
 -5    126   -110
 -4    341   -349
 -3    225    198
 -2    733   -760
 -1    317   -337

H=     5,  K=   14

  0    253   -240
  1    211   -188
  2    370   -351
  3    171    167
  4    -60    -15
  5     90    110
 -8    -60      8
 -7    -60     62
 -6    -59     33
 -5    403   -411
 -4    136   -115
 -3    -54    -95
 -2    268   -271
 -1    103    -68

H=     6,  K=   14

  0    -62     76
  1    -60      5
  2    101     84
  3    -63     57
 -7    -61     -2
 -6    -63    106
 -5    180   -184
 -4    -61    -86
 -3     98    -77
 -2    165    176
 -1    302   -307

H=     7,  K=   14

  L     FO     FC

  0    -65     94
  1    292    294
 -5    161    180
 -4    -64    -45
 -3    168    164
 -2    154   -153
 -1    320    328

H=     0,  K=   15

  1    558    581
  2    217    252
  3    753    755
  4     85    100
  5    331    321
  6     85     57
  7    179   -170
  8    -55    -44
  9    104   -106

H=     1,  K=   15

  0    417    439
  1    128   -150
  2    190    191
  3    -46    -15
  4    288   -283
  5    -51     61
  6    193   -199
  7    -56     44
  8    401   -389
 -9    -57     13
 -8    247    240
 -7    166   -169
 -6    -50     26
 -5     81     63
 -4   1123   1122
 -3    165   -183
 -2    -66    193
 -1    192    185

H=     2,  K=   15

  0    147   -161
  1    601   -592
  2    -46     58
  3    134   -137
  4    -50    -16
  5    510   -507
  6    297    269
  7    193   -197
  8     90    -62
 -9    -57      4
 -8    135    128
 -7    711    705
 -6     93     90
 -5    117   -115
 -4    151    176
 -3    289    338
 -2    177   -167
 -1    263    234

H=     3,  K=   15

  0    322   -343
  1    142   -135
  2    741   -748
  3    -52     -6
  4    194   -193
  5    -57     36
  6    268   -270
  7    149   -117
 -9    -58     -5
 -8    252    268
 -7    141    150
 -6    -52    -64
 -5     90     95
 -4    -49      0
 -3    353   -342
 -2    449   -454

  L     FO     FC

 -1    362    389

H=     4,  K=   15

  0    -51     30
  1    508   -521
  2    -54   -106
  3    -57    -40
  4    -59    -63
  5    172   -146
  6    -61     35
 -9    -60    -13
 -8    -59     24
 -7    -59    -19
 -6     95     67
 -5    268   -256
 -4    -51    -44
 -3    592   -510
 -2    208    203
 -1    619   -636

H=     5,  K=   15

  0    248   -252
  1     85     66
  2    418    429
  3    -60    -98
  4    134   -161
  5    111     71
 -8    -62     37
 -7    151   -127
 -6    264   -257
 -5    126    133
 -4    313   -318
 -3    -54   -101
 -2    267   -252
 -1    -53    -20

H=     6,  K=   15

  0    -61    -40
  1    -61      5
  2    163    168
  3    124    142
 -7    -62    -40
 -6    -61    -30
 -5    121    -99
 -4    -61    -55
 -3    177   -169
 -2     89    121
 -1    466    484

H=     7,  K=   15

  0    355    365
 -5    -67     80
 -4    347    351
 -3    116     99
 -2    198    181
 -1    -64    -33

H=     0,  K=   16

  0    602    604
  1    337   -334
  2    427    441
  3    287   -275
  4    540    550
  5    296   -309
  6    310    292
  7    521   -524
  8    -56    -27
  9    -57     25

H=     1,  K=   16

  0    -44     -5
  1    348    363
  2    511   -496
  3    143   -177

  L     FO     FC

  4    207   -161
  5    -51     45
  6     99    -86
  7    269   -259
  8    178   -150
 -9    222    201
 -8    365    366
 -7    315    308
 -6    191    185
 -5    566    572
 -4    -49     43
 -3    429    427
 -2    362   -459
 -1    334    331

H=     2,  K=   16

  0    341   -369
  1    240   -226
  2    142   -133
  3    200   -182
  4    415   -398
  5    240   -245
  6    489   -463
  7    -56     46
  8    -59     -7
 -9     96     68
 -8    250    253
 -7    159    136
 -6    271    246
 -5    137    -97
 -4     84    -92
 -3    230   -237
 -2    592    571
 -1     70     43

H=     3,  K=   16

  0    427   -415
  1    352   -356
  2    -52    -84
  3    574   -579
  4    173   -160
  5    -57    -83
  6    313    311
  7    317   -288
 -9    155    165
 -8    181   -184
 -7    -55    -58
 -6    -57    -11
 -5    166    111
 -4    560   -575
 -3    382   -415
 -2    222   -203
 -1    142   -159

H=     4,  K=   16

  0    424   -420
  1    232    235
  2    -51      9
  3    203    197
  4    153   -147
  5    515    516
  6    -62    -29
 -8    -61     -5
 -7    363   -345
 -6    389   -389
 -5    174   -169
 -4    300   -299
 -3    420   -432
 -2    311   -307
 -1    301    322

H=     5,  K=   16

  0    364    373
  1    -59     36
  2    269    282
  3    -62     86
```

```
    L     FO      FC

    4    172     157
   -8    -62     -64
   -7    210    -212
   -6    235    -214
   -5    246    -255
   -4    332     323
   -3    -59      78
   -2    173     165
   -1    347    -338

 H=      6,  K=   16

    0    -60     -19
    1    226     223
    2    -64     110
   -7    -63      43
   -6    -61      47
   -5    213     222
   -4    186    -165
   -3    169     151
   -2    -60      61
   -1    215     213

 H=      7,  K=   16

   -4    -65      50
   -3    189     181
   -2    214     212
   -1    -66      97

 H=      0,  K=   17

    1    271    -310
    2    638    -632
    3    228    -227
    4    131    -117
    5    -51      33
    6    911    -913
    7    114      97
    8    106    -109

 H=      1,  K=   17

    0    131     139
    1    310    -285
    2     95     115
    3    881    -866
    4    246    -234
    5     93    -100
    6    220     213
    7    329    -315
    8     91      88
   -9    283     271
   -8    -55     -23
   -7    230     241
   -6    116     -95
   -5     81      75
   -4    126     120
   -3    -47     -33
   -2    -88    -216
   -1    215    -263

 H=      2,  K=   17

    0    480    -467
    1    112    -105
    2    358    -371
    3    135    -139
    4    -52      29
    5    -56      53
    6    108    -126
    7    163     146
   -9    -58     -61
   -8    -56     -19
   -7    -54      44
   -6    143    -166
   -5    -50      14
   -4    249    -244
   -3    -52       6
   -2    303    -303

    L     FO      FC

   -1    443     449

 H=      3,  K=   17

    0    218     198
    1    180    -188
    2    -52      63
    3    338     318
    4    227     227
    5     99     -92
    6    -58      17
    7    347     340
   -9    229    -221
   -8    -59     -30
   -7    168    -187
   -6    217    -292
   -5    628    -640
   -4    131     147
   -3    328    -311
   -2     92      61
   -1    649    -641

 H=      4,  K=   17

    0    487     496
    1    166     194
    2    -59     -18
    3    -59      89
    4    425     424
    5    -63     -30
   -8    576    -553
   -7    189    -174
   -6    244    -248
   -5    124      98
   -4    334    -342
   -3     79      86
   -2    416    -410
   -1    -53      -3

 H=      5,  K=   17

    0    199    -188
    1    359     347
    2    136     142
    3    165     154
    4     97     -32
   -7    -60     -25
   -6    -60    -107
   -5    237    -241
   -4    -60     -50
   -3    358     347
   -2    -58     -33
   -1    -60      71

 H=      6,  K=   17

    0    345     337
    1    -64     -82
    2    -65      43
   -6    160     150
   -5    -63     -55
   -4    242     233
   -3    -62      26
   -2    218     209
   -1    -61     -36

 H=      7,  K=   17

   -2    132    -103

 H=      0,  K=   18

    0    432    -425
    1    504    -580
    2    721    -725
    3    -49      45
    4    -50     -69
    5    141    -130
    6    206    -230
    7    323    -347

    L     FO      FC

    8    -57     -44

 H=      1,  K=   18

    0    118     106
    1    335    -311
    2    491    -474
    3    -51     -25
    4    323    -290
    5    149    -133
    6    224    -214
    7    369     367
    8    242    -194
   -8    134     124
   -7    246    -251
   -6    217    -218
   -5    -51     -64
   -4    225     219
   -3    427    -426
   -2    -83    -260
   -1    507    -519

 H=      2,  K=   18

    0    182     190
    1    227    -209
    2    132     144
    3    130    -118
    4    -52     -57
    5    130    -129
    6    376     361
    7     88      16
   -8    165    -185
   -7    181    -162
   -6    387    -363
   -5    297    -283
   -4    230    -236
   -3    112    -159
   -2    385    -395
   -1    357    -331

 H=      3,  K=   18

    0    285    -272
    1    438     424
    2    -52      75
    3    259     269
    4     85      84
    5    314     295
    6    -61      45
   -8    173    -164
   -7    180    -185
   -6    181    -202
   -5    305    -293
   -4    453    -449
   -3    280     292
   -2     78     -14
   -1    302     314

 H=      4,  K=   18

    0    525     529
    1    -59     -29
    2    426     410
    3    116     127
    4    194     179
    5    319     305
   -8    -64      99
   -7    203    -216
   -6     92     107
   -5    -59      -3
   -4    580     598
   -3    196    -195
   -2    234     219
   -1    -53     -22

 H=      5,  K=   18

    0    -59      85
    1    -58      16

    L     FO      FC

    2    264     269
    3     94      79
    4    -62       6
   -7    374     370
   -6    -61     -67
   -5    316     346
   -4    182     183
   -3    102      96
   -2     88     -87
   -1    440     461

 H=      6,  K=   18

    0    105    -104
    1    -63       0
   -2    149    -134
   -6    202     162
   -5    117     131
   -4    202     165
   -3    -63      71
   -2    -62      57
   -1    205     193

 H=      0,  K=   19

    1    705    -674
    2     96     103
    3    585    -623
    4     74      45
    5    103      92
    6    225     206
    7    156    -158
    8    231     217

 H=      1,  K=   19

    0    378    -390
    1    424     404
    2     83      86
    3    -51     -29
    4     90      62
    5    444     424
    6    -58     -16
    7    -58       5
   -8    258    -244
   -7    -56     -96
   -6    279    -279
   -5    109     111
   -4    620    -610
   -3    -52      68
   -2    239    -369
   -1    356     356

 H=      2,  K=   19

    0    132     105
    1    464     484
    2    370     367
    3    251    -263
    4    -56     -24
    5    400     383
    6    118     108
    7    179     183
   -8    190     184
   -7    557    -558
   -6    -56     -45
   -5    -50      25
   -4    283     297
   -3    -70    -156
   -2    236     240
   -1    292    -288

 H=      3,  K=   19

    0    165     152
    1    131    -132
    2    643     638
    3    287     274
    4    225     235
    5    117    -124
   L     FO      FC

   6    280     270
  -8    222    -209
  -7    373     361
  -6    -57      41
  -5    -59     114
  -4    -56     -72
  -3    -51      19
  -2    135     167
  -1    341     345

H=     4,  K=    19

   0    114      86
   1    560     560
   2    207    -203
   3    118     110
   4    109     -96
   5    -62      40
  -8    -62      46
  -7    156     166
  -6    244     231
  -5    290     284
  -4    -60     -22
  -3    408     403
  -2    -58     -64
  -1    371     392

H=     5,  K=    19

   0    136     140
   1    -60     -36
   2     99     -75
   3    147    -134
  -7    -63      -9
  -6    461     453
  -5    -60     -45
  -4    285     279
  -3    -58       3
  -2    247     242
  -1    147    -157

H=     6,  K=    19

   0    121    -138
   1     95      40
  -5    156     157
  -4    -64     -58
  -3    142     134
  -2    -63      -5
  -1    100     -85

H=     0,  K=    20

   0    177    -199
   1    460     482
   2    -50      28
   3    329     334
   4     81      44
   5    229     223
   6    128    -120
   7    398     401
   8    -58      36

H=     1,  K=    20

   0    564     542
   1    124    -124
   2    358     327
   3    -52       7
   4    112      91
   5    -57     -35
   6    255     246
   7    143     124
  -8    353    -329
  -7    111    -100
  -6    -56     -13
  -5    287     290
  -4    128    -144
  -3    494    -497
  -2    -79     -36
```

```
   L     FO      FC

  -1    158     163

H=     2,  K=    20

   0    261     283
   1    440     430
   2    -53      -7
   3    200     174
   4    -56      45
   5    -57      23
   6    221     228
  -8    117    -115
  -7    139     146
  -6    -55      -3
  -5    213    -226
  -4    177    -199
  -3    561     567
  -2     76     -89
  -1    -50     -35

H=     3,  K=    20

   0    345     347
   1    231     239
   2    -59     -15
   3     89      61
   4     90      78
   5    -60      75
   6    290    -300
  -8    107     103
  -7    -59     -32
  -6    474     494
  -5    178    -184
  -4    356     354
  -3    278     273
  -2    462     465
  -1    166    -137

H=     4,  K=    20

   0    -59      67
   1    328    -333
   2    141     154
   3    248    -224
   4    127     104
  -7    464     456
  -6     88      26
  -5    308     327
  -4    155     147
  -3    184     207
  -2    -58     -83
  -1    133     136

H=     5,  K=    20

   0    164    -162
   1    113      75
   2    277    -287
   3    -63     -69
  -6    -63       6
  -5    206     219
  -4    -59     -45
  -3    -59     -51
  -2    119    -125
  -1    -60      53

H=     6,  K=    20

   0    148    -135
  -4    156     142
  -3    -63     -21
  -2    -63     -35
  -1    241    -255

H=     0,  K=    21

   1    294     294
   2    193     208
   3    539     527
   4    123     137
```

```
   L     FO      FC

   5    -55       8
   6    467     467
   7    144     169

H=     1,  K=    21

   0    340     339
   1    217     201
   2    278    -271
   3    487     465
   4     87      74
   5    259     252
   6    167    -162
   7    198     188
  -7    263    -256
  -6    533     531
  -5    -57     -19
  -4    160     167
  -3    -62     -96
  -2    -71     226
  -1    155     180

H=     2,  K=    21

   0    174     152
   1    171    -181
   2    495     476
   3    268    -271
   4    183    -192
   5    -57     -55
   6    -60      74
  -7    124     152
  -6    100    -111
  -5    -56      10
  -4    294     310
  -3    -71     -68
  -2    122     112
  -1    210     206

H=     3,  K=    21

   0    274    -265
   1    109    -120
   2    184    -183
   3    -57      -8
   4    312    -294
   5    136    -161
  -7    244     252
  -6    229    -227
  -5    303     303
  -4    -60       7
  -3    204     208
  -2    -57     -47
  -1    143     134

H=     4,  K=    21

   0    284    -299
   1    243 .  -257
   2    -61     -62
   3    100      99
   4    371    -353
  -7    -62     -15
  -6    125     123
  -5    241    -225
  -4    166     169
  -3    239    -249
  -2    -58      44
  -1    105    -134

H=     5,  K=    21

   0    193     169
   1    271    -246
   2    -62      24
  -6    208    -216
  -5    -61      29
  -4    -60      67
  -3    -61     -48
  -2    257    -257
```

```
   L     FO      FC

  -1    143    -145

H=     6,  K=    21

  -3    -66      74
  -2    -63      42
  -1    137    -111

H=     0,  K=    22

   0    -51      56
   1    191    -170
   2    516     517
   3    154     193
   4    114      99
   5    -55     -42
   6     88      69
   7    -59      12

H=     1,  K=    22

   0    -53      36
   1    -52      26
   2    189     173
   3    123    -125
   4    333    -310
   5     92    -106
   6    120     116
  -7    130     159
  -6     97    -116
  -5    378     394
  -4     94    -123
  -3    121     130
  -2    114     240
  -1    425     435

H=     2,  K=    22

   0     92     -95
   1    -56      10
   2    276    -251
   3    -56      59
   4    349    -343
   5    120     112
   6    159    -175
  -7    -57       1
  -6    205     197
  -5    132    -147
  -4    224     288
  -3    120     139
  -2    186     165
  -1    -52       8

H=     3,  K=    22

   0    -58      22
   1    225    -199
   2    260     250
   3    365    -351
   4    -60     -52
   5    163    -165
  -7    133     133
  -6    261    -238
  -5    -61      20
  -4    274     252
  -3    -58      75
  -2    184    -158
  -1    405    -406

H=     4,  K=    22

   0    391    -405
   1    -59      -8
   2    190    -191
   3    -61     -12
  -6    -61      23
  -5    195     186
  -4    567    -574
  -3    -59      80
  -2    -58     -39
```

```
   L    FO     FC          L    FO     FC          L    FO     FC          L    FO     FC

  -1   126   -120                                  H=    0, K=   25        H=    2, K=   26
                        H=    5, K=   23
H=    5, K=   22                                      1   266   -293          0   -58     65
                           0   -63     74             2    91     59          1    86    -71
   0   267   -234          1   -63    -17             3   130   -165          2   -60    -56
   1   165    119         -4   239   -225             4   341   -348          3   -59    -25
  -5   125   -113         -3   168    145             5   135   -113          4   213    217
  -4   -62    -69         -2   106   -105                                    -5   -61    -40
  -3   220   -212         -1   133    132          H=    1, K=   25         -4   -78   -168
  -2   -62     12                                                            -3   -58    -79
  -1   104   -108       H=    0, K=   24              0   305   -330         -2   -52     30
                                                      1   359   -363         -1   108     79
H=    0, K=   23           0   -57   -102             2   -56      3
                           1   -75      9             3   375   -358       H=    3, K=   26
   1   307    299          2   254    257             4    95    110
   2   156   -178          3   253   -276             5   239   -318          0   123    153
   3   652    653          4   -57     44            -6   -58    -51          1   122    115
   4   481   -463          5   422   -398            -5   162   -161          2   -61    -84
   5   -55    -13          6   -58      4            -4   390   -375         -4   105    117
   6   238   -240                                    -3   -75   -144         -3   127    159
                        H=    1, K=   24             -2   -63     24         -2   190   -185
H=    1, K=   23                                     -1   111   -143         -1   296    314
                           0   474   -480
   0   317    314          1    88     94          H=    2, K=   25        H=    4, K=   26
   1   163   -167          2   -56     49
   2   153    133          3   282    289             0   213   -187          0   310    310
   3   200   -214          4   571   -541             1   -57     53         -3   135    160
   4   -58    -10          5   105    -98             2   517   -495         -2   378    355
   5   279   -264         -6    84     58             3   127    139         -1   132   -152
   6   233   -231         -5   193   -180             4   -61     60
  -7   188    173         -4   -60     37            -6   -60    -58       H=    0, K=   27
  -6   342    333         -3   152    197            -5   171   -162
  -5   101   -130         -2    84    -98            -4   205   -304          1   226   -286
  -4   396    409         -1   -59    108            -3   -71    -94          2   -78     96
  -3   -63    132                                    -2   440   -433          3   208   -218
  -2   -72    105       H=    2, K=   24             -1   -56     60          4   116    105
  -1   178   -223
                           0   153    153          H=    3, K=   25        H=    1, K=   27
H=    2, K=   23           1   320   -314
                           2   172   -158             0   149    153          0   -59   -104
   0   -56    -71          3   108   -114             1   -59      3          1   -57     44
   1   -57     16          4    99     70             2   -61     67          2   -59    -16
   2   -56    -40          5   -60    -32             3   -61    -13          3   315    290
   3   245   -259         -6    84    -79            -5   189   -191          4   -61    -31
   4    96    102         -5    85   -110            -4   -62    -89         -4   139   -163
   5   249   -224         -4   -71    199            -3   309   -294         -3   -82     99
  -7   160    152         -3   436   -443            -2   330    323         -2   338   -374
  -6   -57    -45         -2   -61   -120            -1   237   -230         -1   272    301
  -5   158    140         -1   -57    -62
  -4   -71   -184                                  H=    4, K=   25        H=    2, K=   27
  -3   -72     21       H=    3, K=   24
  -2   -57     33                                     0   -61     16          0   229    211
  -1   156   -121          0   164   -148             1   109    125          1   -58     38
                           1   245   -228            -4   -63    -54          2   111    131
H=    3, K=   23           2   -58    -51            -3   194    190          3   369    350
                           3   223    212            -2   -63     50         -4   -70     81
   0   439   -451          4    94    100            -1   212    197         -3   -59     17
   1   147    155         -6   334   -341                                    -2   210    190
   2   180   -181         -5   -62    -27          H=    0, K=   26         -1   -59     13
   3   176    185         -4   254   -242
   4   291   -274         -3   -59    -72             0   411   -424       H=    3, K=   27
  -6   152   -176         -2   305   -314             1    89    139
  -5   175   -198         -1    82    -41             2   484   -487          0   214    231
  -4   -61      5                                     3   234   -210          1   114     78
  -3   -55     16       H=    4, K=   24              4   238   -230         -3   138    135
  -2   232   -211                                     5   100     79         -2   -62    100
  -1   312   -329          0   -61    -34                                    -1   201    210
                           1   -61     48          H=    1, K=   26
H=    4, K=   23           2   146   -131                                  H=    0, K=   28
                          -5   237   -240             0   -58     40
   0   186    196         -4   100   -114             1   -58    -62          0    86    106
   1   365   -371         -3   -62    -83             2   212   -190          1   -73     97
   2   298    268         -2   129   -105             3   -61   -107          2   158    122
   3   -62     59         -1    98     95             4   159    152          3   101    121
  -6    87    -52                                    -5   401   -384
  -5   109   -122       H=    5, K=   24             -4    94   -167       H=    1, K=   28
  -4   -64    -77                                    -3   225   -281
  -3   398   -411         -2   344    318            -2   -80    143          0   222    224
  -2   -58    -44         -1   -62      2            -1   371   -379          1   130    158
  -1   164   -162                                                             2   260    244
```

```
   L    FO     FC       L    FO     FC       L    FO     FC       L    FO     FC

   3   -60    -63       2   144    121    H=    0,  K=   29       2   140    123
  -3   -64     95      -3   109     96                            -2   -66     35
  -2   -76    105      -2   133    140       1   201    228       -1    89     86
  -1   -62   -109      -1   384    372       2    94     53
                                                                H=    2,  K=   29
H=    2,  K=   28   H=    3,  K=   28   H=    1,  K=   29
                                                                   0   210    182
   0   130   -154      -1   -61    -13       0   174    187
   1   164    142                            1   191    172
```

FIGURE 14

$[M(DAPPH)(H_2O)_2]^{++}$ COMPLEX IONS

The atomic numbering scheme and thermal ellipsoids for the Co(II) complex are illustrated. The Zn(II) complex is essentially identical except for the metal ion. Hydrogen atoms have been omitted for clarity.

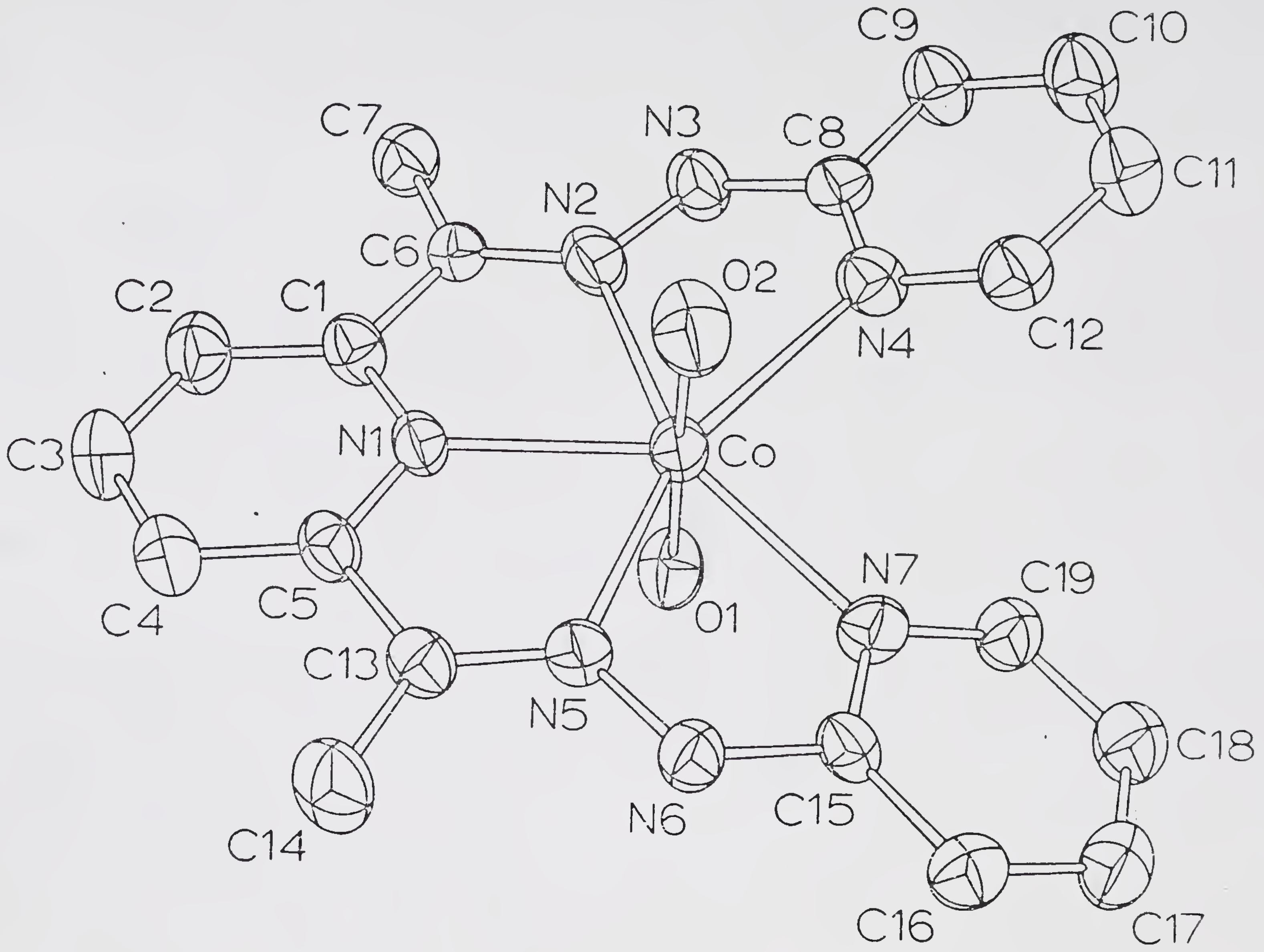
C9
C10
C7
N3
C8
C11
N2
C6
O2
C2
C1
N4
C12
N1
C3
Co
N7
C19
C4
C5
O1
C13
N5
C18
N6
C15
C14
C16
C17

FIGURE 15

A PACKING DIAGRAM FOR $[M(DAPPH)(H_2O)_2]Cl_2$

Dotted lines represent hydrogen bonds listed in Table 36. One half of the unit cell is shown. The atomic numbering scheme and hydrogen atoms are omitted for clarity.

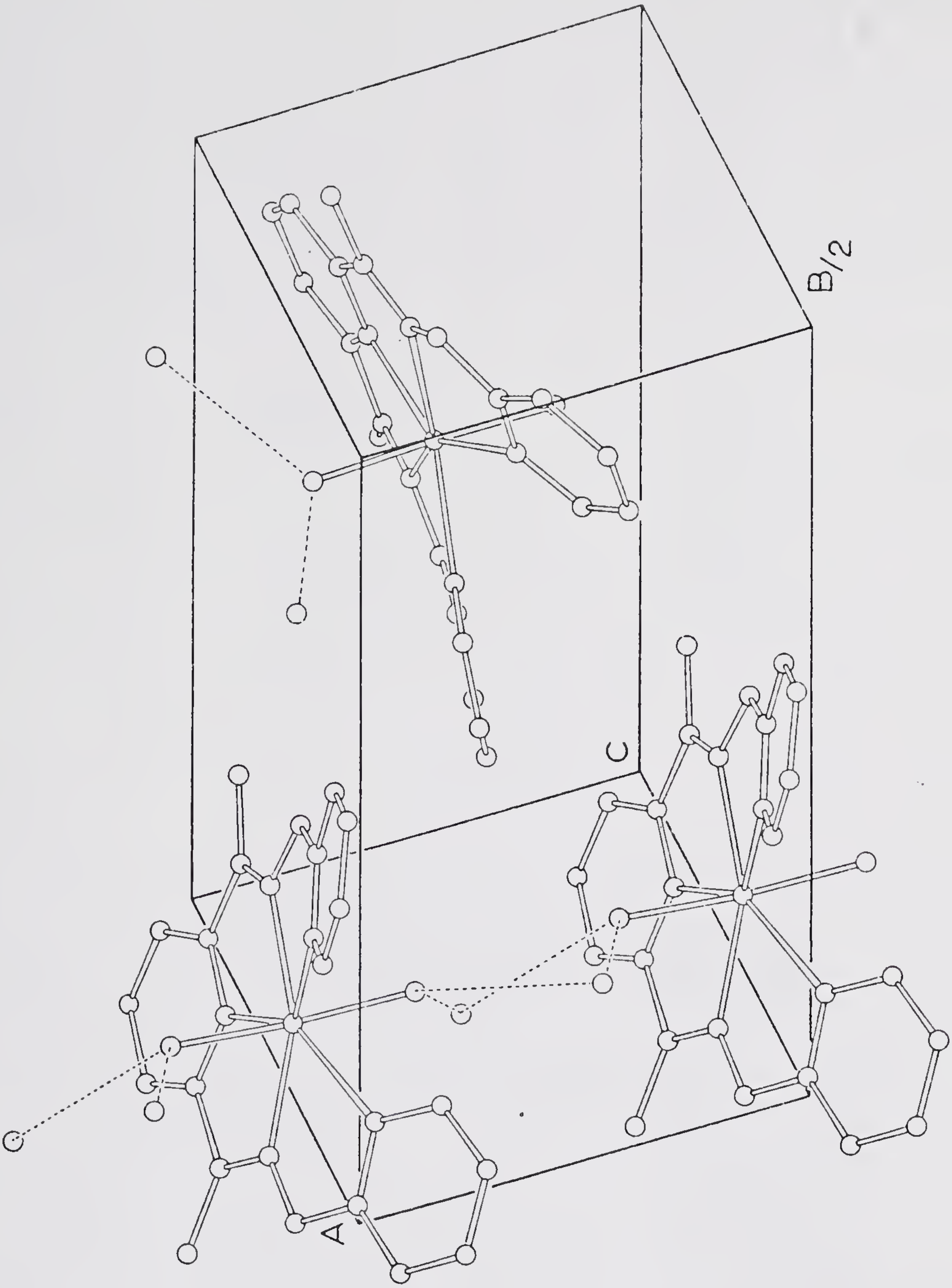
B/2
C
A

Table 39
DATA FOR $[M(DAPPH)(H_2O)_2]^{++}$ IONS

	Co	Zn
M-N(e) average bond distance	2.24(1)Å	2.29(1)Å
M-O(a) average bond distance	2.150(3)	2.104(1)
O(a)-N(e) non-bonded contacts	3.16(7)	3.10(6)
C12-H...H-C19 non-bonded contact	2.56	2.52
Angle between terminal pyridine rings	40.4°	38.3°

Table 40
TORSION ANGLES FOR $[M(DAPPH)(H_2O)_2]Cl_2$ (M=Co,Zn)

	M=Co	Zn
N1-C1-C6-N2	-2.7°	-2.9°
C2-C1-C6-C7	-4.0	-6.2
C7-C6-N2-N3	-0.7	0.5
C6-N2-N3-C8	-9.6	-8.1
N2-N3-C8-N4	11.4	12.5
N2-N3-C8-C9	13.9	13.3
N1-C5-C13-N5	-8.8	-10.4
C4-C5-C13-C14	-12.3	-12.4
C14-C13-N5-N6	0.9	1.6
C13-N5-N6-C15	-9.3	-8.0
N5-N6-C15-N7	9.6	10.5
N5-N6-C15-C16	10.4	11.0

The metal-DAPPH distances are generally longer than previously reported values for similar bonds in complexes of lower coordination number.[23,55,65-67,115] The constraints of the DAPPH ligand are probably the most important factors contributing to these longer distances. However, the fact that the average Co-N and Zn-N distances (2.24(1)Å and 2.29(1)Å, respectively) are longer than those observed in the corresponging DAPSC complexes suggests that steric factors may be important. The non-bonded contacts between the hydrogen atoms bonded to C12 and C19 are 2.56Å and 2.52Å for Co and Zn, respectively, approximately the sum of van der Waals radii of 2.4Å.[74] Therefore, further approach in a more planar arrangement around the metal atoms is inhibited. An examination of the various torsion angles in DAPPH indicates that the ligand is not planar, but has twisted to minimize hydrogen-hydrogen interactions while allowing the donor atoms to bond to the metal ion. Such twisting has been noted in a similar complex containing sulfur donors.[23] The torsion angles about N3 and N6 are large, since these atoms are not strictly conjugated to their neighbors. The angle between the least-squares planes of the terminal pyridine rings is ~39° and aids an increase of H-H contact distances. As in the DAPSC case, the pentagonal planar arrangement of DAPPH nitrogen donors is staggered, while the overall conformation of the ligand is readily discernable in the packing diagram, Figure 15. The angle between the least-squares planes of the donor set and the central pyridine ring is

13.6° for each complex. The terminal pyridine rings are not tilted equally with respect to the central ring. In both cases, a difference of ~6.5° between the dihedral angles of the terminal rings with the central ring exists.

The influence of the ionic radius of the metal ion and the orientation of orbitals must also be considered. The ionic radius of Zn(II) is larger than that of Co(II), and larger metal-ligand bond lengths are observed in the Zn(II) complex. In the case of Zn(II), electrons have been added to the d_{xy} and $d_{x^2-y^2}$ orbitals, both of which are directed at the planar donors, and electron-electron repulsion also contributes to the increased bond lengths.

The metal-axial water bond lengths decrease significantly on going from Co(II) to Zn(II). Once again, nonbonded contacts appear to play an important role in determining these distances. The average contact distances for each compound are not significantly different. However, the metal-ligand in-plane distances are larger for Zn(II), implying that the axial donors are influenced primarily by interaction with the planar donors. This feature has been pointed out previously for the DAPSC complexes, and may be a general property of this class of complexes. The axial water-nitrogen contact distances are identical within experimental error for DAPPH and DAPSC complexes.

The packing diagram illustrates the hydrogen bonding and molecular orientation in the unit cell. Each ionic chloride is hydrogen bonded to two water molecules.

Appropriate data are in Table 36. The lengths of these bonds are shorter than the sum of van der Waals radii,[74] and below the limit within which hydrogen bonds are said to exist.[75] The angles of these bonds are less than 180° which is common for hydrogen bonds.[116]

Structure Solution and Refinement for $Zn(DAPP)\cdot CHCl_3\cdot H_2O$

The zinc atom was located from a sharpened three-dimensional Patterson function. A Fourier synthesis phased only on the zinc atoms revealed the coordination sphere and the chloroform orientations. Subsequent Fourier syntheses established the entire dimeric structure, R=0.21. The trial structure was refined by three full matrix least-squares cycles using isotropic thermal parameters, R=0.13. Then the zinc and chlorine thermal parameters were converted to anisotropic values and the structure was further refined by three least-squares cycles, R=0.093. Three block diagonal least-squares cycles with anisotropic thermal parameters for all atoms reduced R to 0.085. A difference Fourier synthesis revealed the positions of sixteen hydrogen atoms. These were assigned thermal parameters one unit larger than the atoms to which they were bonded. Three block diagonal least-squares cycles holding the hydrogen parameters constant reduced R to 0.080. Since all parameter shifts were less than one-third of their respective estimated standard deviations refinement was terminated.

Results for $[Zn(DAPP)]_2 \cdot 2CHCl_3 \cdot 2H_2O$

The final positional and thermal parameters for the non-hydrogen atoms are listed in Table 41. Probable positional and thermal parameters and bond distances for the hydrogen atoms appear in Table 42. Intramolecular bond distances and angles and short intermolecular contacts are given in Table 43. Least-squares planes and deviations comprise Table 44. The observed and calculated structure factors are listed in Table 45. Figure 16 is an ORTEP[58] diagram of the inner coordination sphere of the dimer. An ORTEP[58] stereo diagram of the entire dimer can be viewed in Figure 17.

Discussion

The inner coordination sphere of the dimer consists of two zinc atoms with distorted octahedral coordination. The numbering scheme is identical to that for DAPPH, except that primed labels designate atoms of the second DAPP ligand. A crystallographic two-fold axis is present perpendicular to the Zn-Zn' and N1-N1' vectors. Thus primed atoms are related to unprimed atoms of the same designation by a two-fold axis. In Figure 16, atoms Zn is shown coordinated to N1, N2, N4, N1', N5', and N7'; while atom Zn' is coordinated to N1, N5, N7, N1', N2', and N4'.

The distorted coordination sphere for each Zn is consistent with other structures[117-124] and with the supposition that the stereochemistry is governed almost entirely by

Table 41
FINAL POSITIONAL AND THERMAL PARAMETERS (x 10^4) FOR THE NON-HYDROGEN ATOMS OF
$Zn(DAPP) \cdot CHCl_3 \cdot H_2O$
WITH THEIR RESPECTIVE ESTIMATED STANDARD DEVIATIONS IN PARENTHESES

ATOM	X	Y	Z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Zn	226(1)	391(1)	1774(1)	32(1)	72(1)	25(1)	4(2)	-6(1)	3(2)
Cℓ1	1931(4)	4424(6)	5104(3)	86(3)	188(8)	61(2)	-36(8)	62(4)	-2(7)
Cℓ2	1420(4)	2106(5)	5450(3)	110(4)	114(5)	49(2)	49(7)	17(4)	17(5)
Cℓ3	554(4)	3535(7)	4632(2)	94(3)	278(10)	28(1)	20(9)	-4(3)	20(6)
N1	889(5)	576(9)	2809(4)	32(4)	60(10)	21(2)	-8(10)	17(5)	-10(8)
N2	547(5)	-1283(9)	2048(4)	35(4)	66(10)	16(2)	37(11)	-8(5)	10(8)
N3	245(6)	-2237(8)	1727(5)	38(4)	56(9)	21(2)	9(11)	-2(5)	-13(9)
N4	-274(5)	-668(9)	1138(4)	26(4)	70(10)	19(2)	-3(10)	-10(5)	5(8)
N5	-24(5)	2206(9)	1738(4)	28(4)	64(10)	15(2)	4(10)	4(5)	-1(8)
N6	499(5)	2959(9)	1582(4)	25(4)	85(11)	19(3)	-22(11)	17(5)	5(9)
N7	1121(5)	1137(9)	1493(4)	21(4)	77(11)	21(3)	16(10)	-4(5)	7(9)
C1	1330(7)	-373(12)	2765(5)	32(5)	84(13)	13(3)	16(14)	7(6)	-10(10)
C2	2061(8)	-289(14)	2957(6)	36(6)	111(16)	26(4)	17(16)	0(7)	17(13)
C3	2332(8)	790(14)	3159(7)	29(5)	112(17)	32(4)	0(16)	-2(7)	19(13)
C4	1897(7)	1789(14)	3196(6)	20(5)	139(18)	28(4)	-3(15)	6(7)	-5(14)
C5	1156(6)	1641(11)	3027(5)	20(4)	76(13)	21(3)	2(12)	17(6)	0(10)
C6	1039(8)	-1473(11)	2469(6)	42(6)	66(13)	20(3)	40(14)	8(7)	18(11)
C7	1314(8)	-2715(12)	2651(6)	54(7)	60(14)	26(4)	14(15)	-22(8)	-1(12)
C8	-193(7)	-1853(12)	1251(5)	29(5)	88(13)	15(3)	3(14)	7(6)	2(10)
C9	-534(8)	-2757(12)	891(6)	44(6)	87(15)	20(3)	-8(15)	-10(7)	-31(11)

Table 41 - continued

ATOM	X	Y	Z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
C10	-977(8)	-2391(13)	403(6)	39(6)	116(17)	20(3)	-5(16)	-10(7)	-16(12)
C11	-1048(8)	-1165(15)	284(7)	41(6)	126(19)	27(4)	7(17)	-12(8)	7(14)
C12	-691(8)	-318(14)	652(6)	50(6)	116(17)	21(3)	14(18)	-12(7)	-23(14)
C13	641(7)	2568(12)	3134(5)	31(5)	86(14)	14(3)	-11(13)	9(6)	-8(10)
C14	838(8)	3920(13)	3096(6)	37(6)	87(15)	27(4)	-18(15)	12(7)	14(12)
C15	1080(6)	2378(12)	1423(5)	20(4)	101(14)	16(3)	-19(13)	-1(6)	-12(10)
C16	1636(6)	3014(13)	1204(6)	20(5)	108(15)	24(3)	-18(14)	4(6)	-12(12)
C17	2231(7)	2432(12)	1050(6)	19(5)	104(15)	26(3)	-23(14)	15(6)	-12(12)
C18	2284(6)	1162(14)	1138(6)	13(4)	132(17)	29(4)	0(14)	-3(6)	-32(13)
C19	1727(7)	599(12)	1347(6)	23(5)	106(16)	22(3)	-16(14)	-10(6)	-8(12)
C20	1183(10)	3569(15)	5237(7)	71(9)	117(18)	26(4)	-12(20)	15(10)	-7(14)
O1	4159(5)	490(8)	3547(4)	44(4)	89(10)	32(3)	-6(11)	14(5)	1(9)

Table 42
POSITIONAL AND THERMAL PARAMETERS (x 10^3) FOR THE HYDROGEN ATOMS OF $Zn(DAPP)\cdot CHCl_3\cdot H_2O$

ATOM	BONDED TO	DISTANCE, Å	X	Y	Z	B(Å^2)
H1	C2	1.01	225	-114	292	6.0
H2	C3	1.18	295	88	315	6.4
H4	C7	0.95	157	-257	302	6.0
H5	C7	0.89	82	-329	265	6.0
H6	C7	0.87	134	-338	245	6.0
H7	C14	1.15	102	410	264	5.7
H8	C14	1.03	119	396	346	5.7
H9	C14	1.00	44	414	334	5.7
H12	C11	1.10	-122	-71	-13	6.9
H13	C12	1.03	-91	45	82	6.8
H14	C16	1.10	155	400	121	5.2
H15	C17	1.05	264	292	87	5.5
H16	C18	1.06	284	106	120	5.8
H17	C19	1.04	176	-30	149	5.3
H18	C20	1.16	105	391	569	7.6
H21	O1	0.85	395	40	326	6.5

Table 43
INTRAMOLECULAR BOND DISTANCES AND ANGLES AND SHORT INTERMOLECULAR CONTACTS FOR $Zn(DAPP)\cdot CHCl_3\cdot H_2O$ WITH THEIR ESTIMATED STANDARD DEVIATIONS IN PARENTHESES

(a) Bond Distances (Å)

Zn-N1	2.590(10)	C2-C3	1.364(21)
Zn-N2	2.032(10)	C3-C4	1.384(21)
Zn-N4	2.036(10)	C4-C5	1.427(18)
Zn-N5'	2.064(10)	C5-C13	1.447(18)
Zn-N7'	2.031(10)	C6-C7	1.515(19)
Zn-N1'	2.390(10)	C8-C9	1.416(19)
Zn-Zn'	3.503(2)	C9-C10	1.395(20)
N1-C1	1.350(16)	C10-C11	1.389(22)
N1-C5	1.360(16)	C11-C12	1.395(22)
N2-N3	1.382(14)	N4-C12	1.362(18)
N2-C6	1.296(17)	C13'-C14'	1.546(19)
N3-C8	1.377(16)	C15'-C16'	1.391(18)
N4-C8	1.343(16)	C16'-C17'	1.366(18)
N5'-C13'	1.287(16)	C17'-C18'	1.423(20)
N5'-N6'	1.362(14)	C18'-C19'	1.343(18)
N6'-C15'	1.346(16)	N7'-C19'	1.355(16)
N7'-C15'	1.385(17)	Cℓ1-C20	1.746(19)
C1-C2	1.411(19)	Cℓ2-C20	1.739(17)
C1-C6	1.475(18)	Cℓ3-C20	1.743(18)

(b) Bond Angles (°)

N1-Zn-N2	71.4(4)	N1-C1-C6	118.0(11)
N1-Zn-N4	148.9(4)	C2-C1-C6	120.8(12)
N1-Zn-N5'	92.8(3)	C1-C2-C3	119.4(13)
N1-Zn-N7'	84.8(4)	C2-C3-C4	120.9(14)
N1-Zn-N1'	89.9(3)	C3-C4-C5	117.6(13)
N2-Zn-N4	78.7(4)	N1-C5-C4	121.5(11)
N2-Zn-N5'	163.9(4)	N1-C5-C13	116.4(11)
N2-Zn-N7'	103.6(4)	C4-C5-C13	121.9(11)
N2-Zn-N1'	101.7(4)	N2-C6-C1	114.9(11)
N4-Zn-N5'	116.3(4)	N2-C6-C7	123.8(12)

Table 43 - continued

(b) continued

N4-Zn-N7'	110.7(4)	C1-C6-C7	121.2(12)
N4-Zn-N1'	88.1(4)	N3-C8-N4	120.3(11)
N5'-Zn-N7'	77.6(4)	N3-C8-C9	117.0(11)
N5'-Zn-N1'	74.2(4)	N4-C8-C9	122.6(11)
N7'-Zn-N1'	150.9(4)	C8-C9-C10	118.1(12)
Zn-N1-C1	97.0(7)	C9-C10-C11	118.8(13)
Zn-N1-C5	122.6(8)	C10-C11-C12	120.4(14)
C1-N1-C5	119.4(10)	N4-C12-C11	121.1(13)
Zn-N2-N3	115.8(7)	C5-C13-C14	120.7(11)
Zn-N2-C6	123.6(9)	C5-C13-N5	116.7(11)
N3-N2-C6	120.5(10)	C14-C13-N5	122.6(11)
N2-N3-C8	112.1(10)	N6'-C15'-N7'	118.8(11)
Zn-N4-C8	112.7(8)	N6'-C15'-C16'	120.7(11)
Zn-N4-C12	128.2(9)	N7'-C15'-C16'	120.5(11)
C8-N4-C12	119.0(11)	C15'-C16'-C17'	121.0(12)
Zn-N5'-N6'	116.0(7)	C16'-C17'-C18'	118.6(12)
Zn-N5'C13'	120.1(8)	C17'-C18'C19'	117.6(13)
N6'-N5'C13'	123.9(10)	N7'-C19'-C18'	125.7(12)
N5'-N6'-C15'	113.6(10)	Cℓ1-C20-Cℓ2	111.2(10)
Zn-N7'-C15'	113.6(8)	Cℓ1-C20-Cℓ3	112.2(10)
Zn-N7'-C19'	129.8(8)	Cℓ2-C20-Cℓ3	110.1(10)
C15'-N7'-C19'	116.6(10)	Zn-N1-Zn'	89.3(3)
N1-C1-C2	121.1(12)		

(c) Short Intermolecular Contacts (Å)

ATOM A	EQUIV.POS.	ATOM B	EQUIV.POS.	DIST
O1	X,Y,Z	N3	½-X,½+Y,½-Z	2.849(14)
O1	X,Y,Z	N6	½-X,Y-½,½-Z	2.896(14)
O1	X,Y,Z	C20	½-X,½-Y,1-Z	3.091(19)

Table 44
LEAST-SQUARES PLANES AND DEVIATIONS FOR Zn(DAPP)·$CHCl_3$·H_2O

The titles of the planes are given, followed by the dihedral angles (°) between the planes. The deviations (x 10^3 Å) of selected atoms from the planes are given. Asterisks denote deviations of atoms used to define the plane. The equations of the planes are of the form ax+by+cz=d, where d is the distance (Å) from the origin.

Plane 1. Plane Through Pyridine Ring of DAP Residue Containing C1-C5.

Plane 2. Plane Through Pyridine Ring Containing C8-C12.

Plane 3. Plane Through Pyridine Ring Containing C15-C19.

Plane 4. Plane Through Pyridine Ring of DAP Residue Containing C1'-C5'.

Plane 5. Plane Through Pyridine Ring Containing C8'-C12'.

Plane 6. Plane Through Pyriding Ring Containing C15'-C19'.

Plane 7. Plane Through Two Zinc Atoms and Bridging Nitrogens.

Dihedral Angles Between Planes

PLANE A	PLANE B	ANGLE	PLANE A	PLANE B	ANGLE
1	2	44.51	3	4	42.35
1	3	35.62	3	5	76.74
1	4	31.95	3	6	15.41
1	5	43.16	3	7	82.29
1	6	42.35	4	5	44.58
1	7	74.02	4	6	35.62
2	3	77.11	4	7	82.29
2	4	42.98	5	6	77.23

Table 44 - continued

PLANE A	PLANE B	ANGLE	PLANE A	PLANE B	ANGLE
2	5	3.70	5	7	88.22
2	6	76.58	6	7	82.29
2	7	88.08			

	PLANE 1	PLANE 2	PLANE 3	PLANE 4	PLANE 5	PLANE 6	PLANE 7
a	-0.2551	0.8348	0.3402	-0.2551	0.8362	0.3401	0
b	-0.2752	-0.0334	-0.1341	0.2752	0.0311	0.1341	1
c	0.9269	-0.5496	0.9307	0.9269	-0.5475	0.9308	0
d	5.4775	-2.0096	6.3145	5.3441	-5.0573	3.9650	0.5350
Zn	-1867	-164	-2581	-1495	2920	-116	-102*
N1	-1*	-596	-56	484	2507	2465	102*
Zn'	1495	-2935	116	1867	155	2582	-102*
N1'	-484	-2516	-2465	1*	580	56	102*

ATOM	DEV.	ATOM	DEV.	ATOM	DEV.	ATOM	DEV.	ATOM	DEV.	ATOM	DEV.
C1	-19*	N4	-11*	N7	8*	C1'	19*	N4'	8*	N7'	-8*
C2	20*	C8	1*	C15	-5*	C2'	-20*	C8'	-2*	C15'	5*
C3	-3*	C9	9*	C16	-7*	C3'	3*	C9'	-4*	C16'	7*
C4	-17*	C10	-10*	C17	15*	C4'	17*	C10'	3*	C17'	-15*
C5	19*	C11	1*	C18	-12*	C5'	-19*	C11'	4*	C18'	12*
		C12	10*	C19	1*			C12'	-10*	C19'	-1*

Table 45

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $Zn(DAPP)\cdot CHCl_3\cdot H_2O$

The structure factors for the reflection (HKL) are listed to the right of the appropriate L value under the corresponding H and K values. FO and FC refer to F_{obs} and F_{calc} respectively.

```
   L    FO     FC

 H=    0,  K=    0

   2   751   -783
   4   135   -128
   6  1994   2237
   8   837   -846
  10   116    -99
  12   218   -215
  14  1014   -933
  16   -72    117
  18   -75     10
  20   247   -267
  22   202    187

 H=    2,  K=    0

   0  1701   2196
   2  1474  -1651
   4   665   -630
   6  2121   2408
   8  2113  -2331
  10   332   -339
  12   620    592
  14   742   -710
  16   102   -108
  18   -74     74
  20   435   -402
  22   -71     48
 -22   190    218
 -20   -77   -182
 -18   121     55
 -16   146    149
 -14   533   -581
 -12   106    131
 -10   482   -516
  -8   -53    -79
  -6   369   -335
  -4   500   -484
  -2   423   -433

 H=    4,  K=    0

   0   269   -226
   2   226   -258
   4   812    806
   6  1098   1115
   8   977   -911
  10  1614   1911
  12   802    774
  14   981   -935
  16   379    337
  18   252    250
  20   432   -400
 -22   -73     80
 -20   212   -220
 -18   275    357
 -16   323    367
 -14   497   -505
 -12   402    421
 -10   194   -170
  -8   588   -655
  -6   514    581
  -4  2096  -3551
  -2   993  -1056

 H=    6,  K=    0

   0   189   -109
   2   137   -176
   4   775    810
   6   375    401
   8   -59     44
  10   581    573
  12   152     99
  14   619   -609
  16   605    577
  18   -73     57
  20   399   -404
 -22   -72     85

   L    FO     FC

 -20   -77   -152
 -18   432    503
 -16   162    168
 -14   -69    -18
 -12   591    620
 -10   196   -196
  -8   197   -218
  -6   849    959
  -4  1444  -1598
  -2   -53     34

 H=    8,  K=    0

   0    85    150
   2  1078  -1056
   4   849    840
   6  1043   -971
   8   341   -341
  10   517    519
  12   197   -158
  14   215   -169
  16   271    281
  18   -76    -72
 -20   -78   -192
 -18   224    247
 -16   155   -209
 -14   438   -429
 -12   385    395
 -10   945   -941
  -8   196    223
  -6  1037   1100
  -4  1153  -1196
  -2   -55     35

 H=   10,  K=    0

   0   337    383
   2   816   -753
   4   517    510
   6   -64    -67
   8   383   -344
  10   720    695
  12   203   -218
  14   -79   -129
  16   316    335
  18   156   -178
 -20   -74    -83
 -18   -75     39
 -16   195   -212
 -14   192    189
 -12   589    564
 -10   643   -634
  -8   594    530
  -6   920    918
  -4   246   -220
  -2   271    280

 H=   12,  K=    0

   0   255   -247
   2   315   -309
   4   412    403
   6   250   -280
   8   300   -329
  10   475    478
  12   -82    -66
  14   -81   -148
  16   134    214
 -18   153    224
 -16   -81    112
 -14   269    253
 -12   -81     18
 -10   537   -560
  -8   451    457
  -6   181    202
  -4   749   -728
  -2   317    260

 H=   14,  K=    0

   L    FO     FC

   0   326   -299
   2   410   -321
   4   494    433
   6   383   -314
   8   177   -145
  10   350    382
  12   219   -238
 -16   212   -239
 -14   -89    -43
 -12   -93    103
 -10   194   -169
  -8   -90    -55
  -6   230   -268
  -4   245   -148
  -2   451    463

 H=   16,  K=    0

   0   257   -200
   2   184    144
   4   358    272
   6   353   -326
   8   183   -191
  10   249    283
 -12   297    268
 -10   346   -286
  -8   211     82
  -6   397    318
  -4   230    155
  -2  -128    -22

 H=    1,  K=    1

   0  1435   1783
   1   180   -261
   2  1223  -1349
   3   952    957
   4   638   -627
   5  2102   2368
   6   937    973
   7  1105  -1085
   8   927   -990
   9   323   -286
  10   451    440
  11   285    321
  12   273    311
  13   359   -343
  14   223   -220
  15   113    126
  16   478    427
  17   -72     11
  18   316    284
  19   -75    -29
  20   219   -167
  21   146    107
  22   121     74
 -22   100     74
 -21   -73    -29
 -20   308   -360
 -19   -75    -59
 -18   141    192
 -17   -72    -20
 -16   122    130
 -15   -68    -30
 -14   437   -436
 -13   116    -74
 -12   113    106
 -11   -57     12
 -10    90    107
  -9   831   -802
  -8   581   -561
  -7   454    429
  -6   460   -364
  -5   -54    -43
  -4   134   -201
  -3   326    347
  -2  1377  -1558
  -1   557    565

 H=    3,  K=    1

   L    FO     FC

   0   689    769
   1   293    266
   2   -51   -112
   3   380    322
   4   569    562
   5   776   -751
   6   118    120
   7  1502  -1555
   8   741   -732
   9   210   -191
  10   914    903
  11   267    218
  12   -61     66
  13   789   -724
  14   443   -414
  15   -72    103
  16   462    445
  17   135    125
  18   183    186
  19   -77     60
  20   117    -64
  21   -74     78
 -22   -71     41
 -21   -73    -65
 -20   326   -379
 -19   -76    -10
 -18   214    235
 -17   159   -189
 -16   250    248
 -15   -68    -46
 -14   453   -457
 -13   264   -233
 -12  1027   1065
 -11   244   -224
 -10   -55    -19
  -9   491    456
  -8   189    248
  -7   446    504
  -6  1425   1597
  -5  1487   1501
  -4   788   -844
  -3   171    -93
  -2   246    253
  -1   139    197

 H=    5,  K=    1

   0   636    624
   1   611   -521
   2  1004  -1095
   3   374   -344
   4   604   -511
   5   169    111
   6   -55     19
   7   139   -166
   8   676   -722
   9   -58     -1
  10   356    347
  11    90   -130
  12   374   -349
  13   449   -418
  14   638   -561
  15   323    271
  16   506    481
  17   -76     23
  18   -77    -48
  19   160   -170
  20   -74    -96
  21   149    110
 -22   -73    -10
 -21   -75    -44
 -20   221   -227
 -19   -76    -55
 -18   -77    106
 -17   126   -153
 -16   -71      8
 -15   184   -156
 -14   404   -448
 -13   296    288
```

```
    L    FO     FC

  -12   605    590
  -11   240   -262
  -10   137   -179
   -9   182    198
   -8   619   -576
   -7    98     86
   -6  1255   1281
   -5  1036   1041
   -4  1503  -1616
   -3   154    -93
   -2   705   -662
   -1   110   -103

H=    7,  K=     1

    0   763    741
    1   494    486
    2   455   -489
    3   504    564
    4   534    568
    5   591    585
    6   -57     -5
    7   185    166
    8   351   -399
    9   -62     66
   10   190    222
   11   -65    -69
   12   -68    -41
   13   -71      0
   14   355   -341
   15   237   -258
   16   145    142
   17   203   -211
   18   111   -116
   19   -74     15
   20   -72     24
  -21   -74     97
  -20   169   -226
  -19   -75     62
  -18   -79     97
  -17   -75     38
  -16   111   -114
  -15   -73     67
  -14   245   -226
  -13   -68     17
  -12   394    387
  -11   248   -276
  -10   546   -561
   -9   359   -349
   -8   236    212
   -7    85    -88
   -6  1382   1380
   -5   -55    -84
   -4   820   -797
   -3   139    155
   -2   560    566
   -1    93    -47

H=    9,  K=     1

    0   729    708
    1   234   -213
    2   809   -762
    3   492    497
    4   552    530
    5   291    282
    6   175   -157
    7   -64     73
    8   458   -492
    9   225    207
   10   519    496
   11   106    -86
   12   128   -144
   13   -75      8
   14   315   -352
   15   -77   -113
   16   122    106
   17   155   -139
   18   -76   -130
  -20   -73    -11

    L    FO     FC

  -19   -76     47
  -18   162    161
  -17   -80   -146
  -16   -77    -86
  -15   -74     40
  -14   -75    -52
  -13   143    -97
  -12   246    241
  -11   228   -204
  -10   353   -351
   -9   685   -702
   -8   333    344
   -7   269   -249
   -6   712    727
   -5   419   -431
   -4   506   -525
   -3   507    456
   -2   368    387
   -1   -58     60

H=   11,  K=     1

    0   144   -151
    1   331   -318
    2   313   -300
    3   332    304
    4   514    529
    5   -68    -74
    6   -69    -52
    7   -72    -76
    8   306   -299
    9   291    242
   10   401    417
   11   115    169
   12   -77     -6
   13   -77    132
   14   -79   -138
   15   -78    -29
   16   -77    162
   17   -74    -23
  -19   -73     86
  -18   -77    101
  -17   110     71
  -16   254   -310
  -15   -78      8
  -14   -80     46
  -13   -78     28
  -12   -77    -38
  -11   126    124
  -10   751   -753
   -9   -73   -103
   -8   214    203
   -7   -67     43
   -6   135   -126
   -5   -65    -28
   -4   476   -502
   -3   -63    -57
   -2   340    329
   -1   -64    -48

H=   13,  K=     1

    0   145   -148
    1   279   -257
    2   -71    -43
    3   -71    -68
    4   626    622
    5   192   -154
    6   312   -294
    7   -89     43
    8   -90   -119
    9   -94    114
   10   368    412
   11   -88    -40
   12   -88    -95
   13   -86    115
   14   -87      2
  -17   -76    -14
  -16   164   -125
  -15   -90   -206

    L    FO     FC

  -14   134    125
  -13   374    392
  -12   137    127
  -11   272    294
  -10   310   -281
   -9   -90     -7
   -8   257    274
   -7   206   -231
   -6   -73     41
   -5   -71     37
   -4   247   -276
   -3   -71     14
   -2   539    505
   -1   129   -155

H=   15,  K=     1

    0   472   -332
    1  -128     20
    2  -128    -46
    3  -128     82
    4   418    362
    5  -127   -117
    6   367   -359
    7  -126    -66
    8  -124   -120
    9  -125    -67
   10   244    294
   11  -121    -39
  -15   -99   -118
  -14   165    151
  -13   293    324
  -12   167    184
  -11  -128   -161
  -10   488   -323
   -9   247   -186
   -8  -130     98
   -7   298    255
   -6  -129    -29
   -5  -127     15
   -4   239   -115
   -3  -127    -70
   -2   238    129
   -1   209   -124

H=    0,  K=     2

    0   278   -186
    1   352   -302
    2   609   -649
    3   304    314
    4   237    239
    5  1271   1283
    6   667    687
    7   168   -183
    8   -52    -19
    9   421    415
   10   541    537
   11   347    305
   12   303    303
   13   340   -341
   14   299    284
   15   141   -133
   16   170    193
   17   149   -177
   18   175    152
   19   166   -185
   20   256   -210
   21   -72     65
   22   -71     18

H=    2,  K=     2

    0    82    -59
    1   585   -547
    2   262   -275
    3   176    204
    4   -54     23
    5   -53     89
    6   -52    -58

    L    FO     FC

    7   784   -742
    8   567   -575
    9   574    548
   10   349    309
   11   634    569
   12   212   -182
   13   106   -114
   14   400   -381
   15   -70     36
   16   145    151
   17   119    114
   18   -73     53
   19   -75     26
   20   114     64
   21   109     83
  -22   -72     56
  -21   -72    -71
  -20   293   -298
  -19   217    199
  -18   268    283
  -17   -73     85
  -16   202    186
  -15   171    138
  -14   219   -239
  -13   -63     69
  -12   430    453
  -11   349   -381
  -10   241   -218
   -9   267   -278
   -8   -53    -98
   -7   808   -767
   -6   374   -316
   -5   538   -494
   -4   646   -675
   -3   897   -904
   -2   335   -363
   -1  1365  -1374

H=    4,  K=     2

    0   857    861
    1   711   -754
    2   459   -474
    3   129    218
    4   409    434
    5   211   -143
    6   -54     63
    7   520   -474
    8   448   -495
    9   861    845
   10   141    131
   11   155    158
   12   415   -375
   13   -66      1
   14   297   -281
   15   654    599
   16   468    415
   17   120   -116
   18   -76    -47
   19   -76     74
   20   185    150
   21   124    105
  -22   -71      9
  -21   110   -144
  -20   154   -178
  -19   291    299
  -18   -76    -95
  -17   119    -93
  -16   -71     40
  -15   183   -159
  -14   599   -619
  -13   791    804
  -12   248    262
  -11   -60    -15
  -10   310   -323
   -9   412    430
   -8   454   -476
   -7   186    196
   -6   546    630
   -5   322    294
   L     FO      FC

  -4    280     213
  -3     88      19
  -2    534     478
  -1    326    -330

H=      6,  K=     2

   0    136     211
   1    560    -617
   2    388    -429
   3     78      13
   4    161     169
   5    237    -249
   6    -56     -32
   7    593    -541
   8    448    -444
   9    -61      93
  10    408     399
  11    106      59
  12    -65     -23
  13    -69      90
  14    265    -253
  15    195     204
  16    160     129
  17    319    -316
  18    220    -241
  19    155     127
  20    168     163
 -21    -72     -74
 -20    112    -137
 -19    -76      22
 -18    -77     151
 -17    -76    -109
 -16    -73     -54
 -15    -73    -101
 -14    195    -164
 -13    642     675
 -12    387     427
 -11    123    -157
 -10    145      95
  -9    224    -247
  -8    436     409
  -7    625     687
  -6    670     724
  -5    160     146
  -4    -53     -65
  -3    588    -545
  -2    441     453
  -1    364    -404

H=      8,  K=     2

   0    218    -201
   1    239    -237
   2    656    -706
   3    264     275
   4    427     457
   5    -59     -23
   6    -61     -42
   7    300    -319
   8    169    -201
   9    164     211
  10    535     557
  11    269    -243
  12    -72     -63
  13    121      60
  14    254    -264
  15    -76      97
  16    -75      41
  17    206    -179
  18    148    -164
  19    122     161
 -20    168    -144
 -19    -76      12
 -18    179     197
 -17    184    -215
 -16    113    -105
 -15    -75      13
 -14    190    -205
 -13    -73     108
```

```
   L     FO      FC

 -12    338     368
 -11    113     -67
 -10    178    -232
  -9    130    -154
  -8    533    -538
  -7    650     636
  -6    169     193
  -5    402    -282
  -4    826    -870
  -3    191     228
  -2    -56     -39
  -1    641     587

H=     10,  K=     2

   0    367     362
   1    546    -552
   2    -61      -1
   3    300   . 272
   4    392     416
   5    124     130
   6    181    -189
   7    407    -405
   8    132    -131
   9    -70    -105
  10    430     437
  11    134    -150
  12    -78    -108
  13    134     152
  14    -76      -4
  15    -76      61
  16    -75     119
  17    -73     -51
 -19    -72      33
 -18    152     191
 -17    184    -209
 -16    161    -194
 -15    200     252
 -14    -77      35.
 -13    -75      11
 -12    150     121
 -11    -72      32
 -10    256    -252
  -9    -68     -33
  -8     99      40
  -7    335     298
  -6    300     305
  -5    -63     -36
  -4    211    -214
  -3    467     486
  -2    151     151
  -1    136     164

H=     12,  K=     2

   0    123      80
   1    348    -323
   2    409    -409
   3    309     294
   4    245     233
   5    234    -193
   6    274    -277
   7    -82    -149
   8    170    -187
   9    -81      55
  10    166     179
  11    -83    -105
  12    -82    -150
  13    132      98
  14    -80     137
  15    -77     -37
 -18    -77      50
 -17    -81    -161
 -16    223    -253
 -15    -81      43
 -14    -82     127
 -13    118    -104
 -12    182     199
 -11    -83    -164
 -10    349    -331
```

```
   L     FO      FC

  -9    119     139
  -8    286     285
  -7    196    -249
  -6    159     177
  -5    -73    -165
  -4    359    -352
  -3    218     188
  -2    437     428
  -1    197    -202

H=     14,  K=     2

   0   -104    -113
   1   -102       9
   2    194    -145
   3    303     309
   4    403     344
   5    163    -127
   6    221    -167
   7   -106     164
   8    192    -199
   9   -103     -47
  10   -102     115
  11    155    -183
  12    156    -105
  13    -97      55
 -15   -101     -55
 -14   -103     195
 -13   -105     194
 -12   -104    -178
 -11    175    -142
 -10    248    -267
  -9    249     196
  -8    324     307
  -7    152    -174
  -6   -104     -79
  -5   -104      79
  -4    283    -213
  -3    488     396
  -2    223     171
  -1    264    -219

H=     16,  K=     2

 -12   -122     -12
 -11   -123    -102
 -10    189    -150
  -9   -124      67
  -8    527     415
  -7   -123      46
  -6    329    -291

H=      1,  K=     3

   0    651     682
   1    121    -170
   2    206     184
   3    253     216
   4    300     311
   5    128     140
   6    582     628
   7    500    -503
   8    601    -589
   9    558     545
  10    361     329
  11    343     354
  12    -63     -12
  13    128    -142
  14    364    -329
  15    240     230
  16    -72     -64
  17    -75      33
  18    -75      -3
  19    -72     -26
  20    262    -205
  21    345     302
 -21    154    -206
 -20    230    -224
 -19    -74      26
 -18    274     274
```

```
   L     FO      FC

 -17    -76    -157
 -16    -71     -52
 -15    267    -281
 -14    382    -369
 -13    398     426
 -12    358     392
 -11    -61      21
 -10    217    -240
  -9    107     103
  -8    432    -418
  -7    821     814
  -6    268    -194
  -5    545     495
  -4    284    -298
  -3    -55      44
  -2    238    -234
  -1    763     799

H=      3,  K=     3

   0    888     933
   1    232    -308
   2    597     523
   3    -53      44
   4    487     519
   5    130     113
   6    861     891
   7    564    -540
   8    683    -671
   9    555     569
  10    -61      96
  11    568    -547
  12    -64     -65
  13    283    -287
  14    508    -456
  15    169     105
  16    -73      66
  17    376    -370
  18    143    -141
  19    -74     -61
  20    109     -77
  21    175     173
 -21    -74    -109
 -20    107     103
 -19    173     202
 -18    198     167
 -17    196    -213
 -16    -72      42
 -15    -71      62
 -14    406    -411
 -13    571     581
 -12    690     707
 -11    471    -485
 -10    344    -368
  -9    -58      21
  -8    559    -582
  -7    243     238
  -6    333     310
  -5    379    -427
  -4    129    -150
  -3    398    -385
  -2    -54      65
  -1    132     130

H=      5,  K=     3

   0    340     325
   1    108      86
   2    353    -402
   3    382     373
   4    173     164
   5    442     415
   6    313     319
   7    443    -430
   8    479    -450
   9    -63     132
  10    226     226
  11    176    -168
  12    187     171
  13    -72     -42
```

```
   L     FO     FC

  14    358   -333
  15    176    171
  16    253    253
  17    580   -554
  18    258   -251
  19    -75     61
  20    -71     63
 -21    -73    -63
 -20    -75    114
 -19    165    159
 -18    -76     12
 -17    185   -190
 -16    141   -127
 -15    114   -133
 -14    -70     48
 -13    175    165
 -12    -67    -70
 -11    765   -772
 -10    543   -512
  -9    -60    -52
  -8    -58    -14
  -7    -57     83
  -6    244    232
  -5    628   -694
  -4    659   -681
  -3    263    279
  -2    652   -586
  -1    455    422

H=     7,  K=     3

   0     81     -7
   1    616   -605
   2    953   -960
   3    810    817
   4    607    603
   5    117   -118
   6    507    515
   7    261   -258
   8    -62    -26
   9    306    333
  10    513    503
  11    -68    -71
  12    285    258
  13    144    150
  14    170   -130
  15    194    168
  16    290    284
  17    335   -340
  18    169   -168
  19    126    143
 -20    125   -104
 -19    124    117
 -18    209    239
 -17    117   -132
 -16    165   -167
 -15    -75     42
 -14    -73      3
 -13    283    290
 -12    -68     86
 -11    280   -264
 -10    120   -128
  -9    410    410
  -8    404    374
  -7    494    542
  -6    247   -195
  -5    396   -391
  -4    831   -841
  -3    977   1002
  -2    256    261
  -1    223    210

H=     9,  K=     3

   0    454   -433
   1    788   -798
   2    551   -556
   3    603    598
   4    765    715
   5    201   -202
```

```
   L     FO     FC

   6    -65    -17
   7    287   -266
   8    331   -323
   9    410    368
  10    565    517
  11    160   -139
  12    -76    -81
  13    -77    154
  14    -78     88
  15    270    274
  16    -76     69
  17    161   -165
 -19    -75     46
 -18    181    185
 -17    148   -154
 -16    -77     33
 -15    -78     44
 -14    -77     83
 -13    -76     12
 -12    229    225
 -11    186   -218
 -10    -70     14
  -9    -68    -46
  -8    -66    -16
  -7    -64     46
  -6    113    106
  -5    668   -690
  -4    195   -205
  -3    131    132
  -2    249    239
  -1    403   -401

H=    11,  K=     3

   0    238   -215
   1    193   -187
   2    344   -343
   3    681    701
   4    202    193
   5    306   -308
   6    485   -466
   7    111     83
   8    190   -205
   9    261    253
  10    364    411
  11    334   -386
  12    304   -370
  13    216    244
  14    -77    118
  15    125    116
  16    -76    170
 -18    -75    107
 -17    133   -183
 -16    -79    -39
 -15    176    214
 -14    -79    -37
 -13    -79    -50
 -12    -80     77
 -11    141   -119
 -10    133   -142
  -9    191    129
  -8    -72     94
  -7    138   -100
  -6    155    165
  -5    219   -219
  -4    327   -327
  -3    468    468
  -2    332    328
  -1    152   -163

H=    13,  K=     3

   0    -73     32
   1    -89   -139
   2    440   -415
   3    346    297
   4    272    279
   5    226   -242
   6    194   -230
   7    -90    -13
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```
   L     FO     FC

   8    -92    -90
   9    150     86
  10    -91     94
  11    275   -388
  12    138   -205
  13    -85    103
 -16    -85    -11
 -15    142    189
 -14    -88    -30
 -13    -88    -31
 -12    159    110
 -11    -93   -101
 -10    -92     24
  -9    214    248
  -8    136     56
  -7    -90   -150
  -6    171    189
  -5    -87     77
  -4    -88    -64
  -3    258    250
  -2    332    316
  -1    176   -184

H=    15,  K=     3

   0   -129    -68
   1    199    154
   2   -126    -34
   3   -129     26
   4   -130    191
   5    212   -258
   6   -129   -185
   7    271    288
   8   -125     27
   9   -123    -20
  10   -121     52
 -13   -122    -70
 -12   -122      3
 -11   -128   -143
 -10   -126    -99
  -9    352    277
  -8    216    162
  -7    344   -313
  -6    237   -194
  -5   -128    -14
  -4   -126     43
  -3    300    220
  -2   -130    137
  -1    431   -372

H=     0,  K=     4

   0    798    770
   1    980  -1011
   2    403   -392
   3    481   -432
   4    512   -494
   5    491    454
   6    268    251
   7    980   -991
   8    520   -558
   9    511   -456
  10    108    -90
  11    174    150
  12    461    434
  13    240   -202
  14    104   -138
  15    285    255
  16    120    131
  17    -75      2
  18    243    250
  19    115    -66
  20    167   -161
  21    227    194

H=     2,  K=     4

   0    455    459
   1   1701  -1758
   2    687   -705
```

```
   L     FO     FC

   3   1011    932
   4    648   -640
   5    132    137
   6    635    587
   7    924   -871
   8    977   -947
   9    349    338
  10     97     56
  11    195    215
  12    344    352
  13    200   -224
  14    193   -169
  15    216    164
  16    268    265
  17    -76    -70
  18    140    154
  19    -75    -24
  20    198   -162
 -21    176   -193
 -20    258   -259
 -19    -76     94
 -18    114    131
 -17    209   -215
 -16    -75    115
 -15    207   -180
 -14    372   -359
 -13    163    189
 -12    690    690
 -11    342   -325
 -10    -63    -94
  -9     86    -34
  -8    -60     37
  -7    467    485
  -6    570    571
  -5    914   -904
  -4    482   -492
  -3    -54     43
  -2    265   -285
  -1    368   -303

H=     4,  K=     4

   0    486    503
   1    356   -349
   2    526   -496
   3   1208   1279
   4    180    172
   5    592    560
   6    640    586
   7    567   -560
   8    770   -716
   9    824    855
  10    171    155
  11    345   -327
  12    330    315
  13    481   -432
  14    401   -363
  15    310    291
  16    245    200
  17    267   -223
  18    -76    -75
  19    -76   -120
  20    -71    -52
 -20    124   -115
 -19    147    146
 -18    -74      3
 -17    -77     49
 -16    -76    -41
 -15    -74     24
 -14    233   -212
 -13    255    235
 -12    508    532
 -11    438   -418
 -10    159    145
  -9    145    183
  -8    -60     21
  -7    555    550
  -6    597    644
  -5    206   -229
  -4    509   -509
```

```
   L     FO     FC

  -3    435    422
  -2    308   -276
  -1    717    740

H=      6,  K=    4

   0    762    772
   1    420   -458
   2    533   -556
   3    286    354
   4    381    409
   5    156   -176
   6    395    372
   7    489   -520
   8    597   -613
   9    316    338
  10    117    112
  11    567   -578
  12    -70     36
  13    109   -119
  14    553   -513
  15    298    277
  16    385    255
  17    298   -289
  18    119    -73
  19    -71    -57
 -20    -73   -103
 -19    -76     93
 -18    113    125
 -17    -75    -13
 -16    194   -206
 -15    124   -122
 -14    -74     -4
 -13    -72     38
 -12    116    131
 -11    510   -539
 -10    -66    -47
  -9    -65    104
  -8    141    119
  -7     96    -86
  -6    406    419
  -5    457   -471
  -4    -58    -21
  -3    859    839
  -2    -58    -22
  -1    286   -245

H=      8,  K=    4

   0    -62    102
   1    399   -399
   2    497   -489
   3    560    578
   4    292    282
   5    235   -224
   6    -67    -70
   7    161   -130
   8    460   -438
   9    539    538
  10    211    197
  11    198   -191
  12    -76   -150
  13    -77     15
  14    -79   -123
  15    376    385
  16    168    189
  17    288   -298
 -19    -75     22
 -18    153    172
 -17    223   -187
 -16    195   -229
 -15    -74      4
 -14    146   -130
 -13    155    190
 -12    -72     21
 -11    392   -374
 -10    212   -235
  -9    104    -74
  -8    119    125
  -7    211    220
```

```
   L     FO     FC

  -6    275    262
  -5    305   -314
  -4    108      1
  -3    657    656
  -2    149    130
  -1    392   -360

H=     10,  K=    4

   0    -68     -2
   1    -68    -37
   2    288   -271
   3    470    423
   4    216    224
   5    528   -515
   6    -72    -15
   7    477    435
   8    178   -175
   9    135    169
  10    383    420
  11    178   -230
  12    301   -349
  13    -80     81
  14    -74     20
  15    138    167
  16    -77     81
 -18    -75    111
 -17    113    -87
 -16    121   -148
 -15    317    365
 -14    -77    -57
 -13    124    104
 -12    124     96
 -11    189   -173
 -10    273   -291
  -9    334    296
  -8    -72    -14
  -7    -70     20
  -6    291    271
  -5    332   -324
  -4    310   -315
  -3    316    330
  -2    212    238
  -1    134   -167

H=     12,  K=    4

   0    132     72
   1    391   -384
   2    195   -201
   3    427    478
   4    324    359
   5    356   -387
   6    -83      1
   7    171    173
   8    -81     22
   9    169    168
  10    -82    124
  11    381   -490
  12    144   -203
  13    155    288
  14    -77     20
 -16    -78     -9
 -15    118    112
 -14    -79    -36
 -13    -90    -71
 -12    -84    111
 -11    243   -267
 -10    247   -239
  -9    219    236
  -8    -81    -26
  -7    356   -345
  -6    182    201
  -5    384   -416
  -4    386   -376
  -3    366    364
  -2    418    369
  -1    113    -73

H=     14,  K=    4
```

```
   L     FO     FC


   0   -107    115
   1   -107    106
   2    274   -267
   3   -105    137
   4    351    356
   5   -104   -100
   6    189   -181
   7   -104    -24
   8   -101     16
   9   -102    146
  10    142    158
  11    150   -213
 -14   -101    -22
 -13   -102     46
 -12   -102    108
 -11   -104     -3
 -10    177   -142
  -9    268    235
  -8   -106    -23
  -7    193   -204
  -6   -106     45
  -5   -108    133
  -4    180   -207
  -3    254    265
  -2    199    193
  -1    229   -226

H=      1,  K=    5

   0    443    466
   1    598   -592
   2    170    133
   3   1017   1006
   4    267   -258
   5    664    667
   6    -60     71
   7    132   -161
   8    707   -655
   9    387    395
  10    -65    -45
  11    215    198
  12    -68     52
  13    271   -267
  14    334   -348
  15    285    277
  16    295    276
  17    173   -140
  18    -74     60
  19    156   -106
  20    116   -135
 -20    191   -208
 -19    187    225
 -18    -74     56
 -17    185    196
 -16    -76    104
 -15    182   -170
 -14    194   -188
 -13    493    491
 -12    -70     74
 -11    -68    -30
 -10    116    -63
  -9    380   -389
  -8    322   -344
  -7    731    709
  -6    698    721
  -5    554   -562
  -4    417    410
  -3    277   -246
  -2    170   -163
  -1    530    554

H=      3,  K=    5

   0    133    102
   1   1279  -1289
   2    360   -369
   3    337    333
   4    659   -624
   5    -60    -58
```

```
   L     FC     FC

   6    248    257
   7    634   -617
   8    140    116
   9    646    574
  10    117    -70
  11    -71     -2
  12    112    107
  13    178    -87
  14    215   -194
  15    316    310
  16    301    277
  17    -76    -64
  18    -75     -7
  19    141    -70
 -20    182   -225
 -19    261    255
 -18    142    100
 -17    -76    -31
 -16    -77     14
 -15    -76   -119
 -14    127   -112
 -13    458    427
 -12    308    284
 -11    151   -197
 -10    -67     62
  -9    290   -295
  -8    -61    -13
  -7    873    873
  -6    286    295
  -5    587   -645
  -4    -58    -22
  -3    630   -623
  -2    417   -404
  -1    287    243

H=      5,  K=    5

   0    418    391
   1    817   -851
   2    312   -303
   3    198   -139
   4    320    263
   5    432    397
   6    578    577
   7    358   -339
   8    -66     -1
   9    600    561
  10    151    163
  11    -72    -25
  12    117     55
  13    -74     34
  14    145   -147
  15    372    342
  16    -76     53
  17    -75    -22
  18    -75    -67
 -19    -75    -13
 -18    134    167
 -17    129   -105
 -16    -78    -56
 -15    122   -105
 -14    -74    -13
 -13    258    257
 -12    390    396
 -11    514   -473
 -10    202   -188
  -9    -67     19
  -8    220   -235
  -7    477    456
  -6    187    170
  -5    571   -581
  -4    329   -335
  -3    -61     16
  -2    217   -246
  -1    -60    -52

H=      7,  K=    5

   0    402    385
   1    287   -304
```

L	FO	FC
2	170	-160
3	367	402
4	-65	19
5	-66	47
6	209	191
7	410	-394
8	236	-219
9	279	229
10	177	174
11	-77	-129
12	-77	-49
13	-78	-33
14	141	-145
15	234	180
16	-76	39
17	134	-165
-19	-72	74
-18	-75	84
-17	-74	3
-16	-77	-111
-15	-77	66
-14	-76	-81
-13	335	322
-12	-76	115
-11	234	-265
-10	320	-305
-9	369	369
-8	233	-215
-7	476	503
-6	171	171
-5	349	-340
-4	196	-215
-3	984	968
-2	90	-7
-1	97	-76

H= 9, K= 5

L	FO	FC
0	277	263
1	387	-396
2	403	-423
3	227	241
4	103	41
5	529	-507
6	125	-134
7	140	-141
8	186	-199
9	-75	-37
10	271	320
11	-78	-135
12	152	-134
13	182	-208
14	-74	15
15	210	221
16	-76	135
-17	187	-162
-16	-77	-108
-15	-77	48
-14	115	-81
-13	136	161
-12	173	175
-11	294	-317
-10	134	-137
-9	-76	72
-8	114	50
-7	-72	-6
-6	416	390
-5	347	-342
-4	298	-297
-3	559	573
-2	132	127
-1	190	-191

H= 11, K= 5

L	FO	FC
0	258	207
1	310	-289
2	306	-322
3	524	580
4	-77	-24
5	400	-421
6	-79	57
7	178	178
8	129	-140
9	-79	68
10	-79	125
11	187	-224
12	-75	-2
13	153	174
14	-74	-87
-16	-76	-30
-15	-76	84
-14	-77	-23
-13	-80	125
-12	165	205
-11	241	-263
-10	-80	14
-9	255	248
-8	-78	-13
-7	-79	-59
-6	182	190
-5	163	-180
-4	227	-198
-3	476	470
-2	-73	-45
-1	-74	-66

H= 13, K= 5

L	FO	FC
0	-92	1
1	-91	-121
2	-89	-32
3	255	303
4	187	204
5	-93	-108
6	-92	-125
7	138	-139
8	-89	-42
9	271	333
10	-87	23
11	134	-276
-14	-84	89
-13	141	170
-12	-88	60
-11	-89	-94
-10	145	-221
-9	166	146
-8	-90	21
-7	149	-122
-6	-92	84
-5	135	-95
-4	131	-190
-3	169	190
-2	-90	114
-1	-91	-32

H= 15, K= 5

L	FO	FC
0	-123	128
1	-127	173
2	-124	-57
3	177	1
4	-122	91
5	-122	-85
6	-123	-48
7	-121	33
-10	-119	-96
-9	177	75
-8	-122	151
-7	-123	-75
-6	-122	78
-5	-126	-68
-4	-128	-196
-3	-129	133
-2	-126	132
-1	-129	-216

H= 0, K= 6

L	FO	FC
0	596	-549
1	647	-686
2	-60	20
3	599	585
4	229	246
5	350	350
6	118	-118
7	543	-531
8	110	-104
9	342	335
10	-70	-78
11	-72	53
12	123	-66
13	476	-470
14	-75	-31
15	-77	115
16	-74	10
17	154	-157
18	-73	-38
19	113	6

H= 2, K= 6

L	FO	FC
0	113	102
1	499	-495
2	335	338
3	534	491
4	-63	91
5	101	122
6	191	-157
7	635	-629
8	280	273
9	250	263
10	-73	-62
11	228	-209
12	140	-142
13	388	-352
14	-78	-96
15	-78	20
16	129	132
17	-75	-48
18	-74	-50
-19	-72	56
-18	-73	47
-17	-77	-104
-16	-76	-91
-15	420	-400
-14	-77	84
-13	144	163
-12	-73	10
-11	218	-194
-10	-70	-43
-9	526	-490
-8	-68	-10
-7	488	456
-6	141	138
-5	257	-269
-4	114	112
-3	105	76
-2	98	98
-1	907	939

H= 4, K= 6

L	FO	FC
0	-63	-31
1	391	-369
2	194	-197
3	348	359
4	-67	97
5	124	140
6	-67	-67
7	660	-648
8	197	151
9	490	475
10	201	-188
11	-73	-4
12	218	-226
13	-75	-54
14	133	140
15	168	119
16	-74	-39
17	125	-145
-18	-74	26
-17	234	-254
-16	-74	-83
-15	215	-233
-14	211	185
-13	450	444
-12	113	74
-11	171	-166
-10	246	-255
-9	-71	20
-8	-65	-74
-7	839	839
-6	167	133
-5	-65	-22
-4	121	-130
-3	477	496
-2	259	214
-1	286	330

H= 6, K= 6

L	FO	FC
0	198	188
1	491	-513
2	182	-177
3	271	296
4	-67	69
5	-69	-79
6	247	234
7	331	-308
8	-72	-6
9	372	371
10	224	225
11	-75	83
12	-76	-35
13	142	-108
14	-75	38
15	-76	110
16	-74	-107
-18	-72	-39
-17	-73	-67
-16	-75	65
-15	177	-181
-14	-76	-53
-13	483	488
-12	-75	-88
-11	342	-363
-10	133	-108
-9	127	-101
-8	160	-148
-7	351	343
-6	-70	-23
-5	742	-749
-4	396	-374
-3	142	144
-2	-66	-86
-1	353	-352

H= 8, K= 6

L	FO	FC
0	-70	13
1	189	-169
2	-72	-103
3	627	637
4	111	107
5	128	-127
6	192	204
7	-76	-80
8	130	93
9	191	215
10	126	130
11	-76	-53
12	-77	-32
13	-76	-62
14	-73	22
15	139	217
-17	169	-138
-16	-74	101
-15	140	-119
-14	-76	63

```
  L    FO    FC

 -13   281   295
 -12   116    46
 -11   523  -510
 -10   135   138
  -9   156  -154
  -8   -75   -26
  -7   168   157
  -6   215  -184
  -5   549  -542
  -4   105    53
  -3   289   279
  -2   109   145
  -1   -69   -14

H=   10,  K=    6

   0   -75   -59
   1   230  -252
   2   123  -113
   3   369   387
   4   -76   -44
   5   137  -173
   6   -78   -82
   7   -78   -45
   8   -80  -120
   9   -78    44
  10   -77    98
  11   150  -170
  12   -78    97
  13   -74    60
 -15   -73    51
 -14   -75   -14
 -13   220   244
 -12   -78    -7
 -11   297  -316
 -10   -79    65
  -9   191   177
  -8   -78    10
  -7   267   275
  -6   -78   -82
  -5   267  -283
  -4   -77    54
  -3   421   423
  -2   202  -198
  -1   169   166

H=   12,  K=    6

   0   -83  -107
   1   215  -304
   2   -83   143
   3   204   275
   4   180  -244
   5   -80    14
   6   -81  -110
   7   131  -171
   8   -79   153
   9   -81   112
  10   -78   -89
  11   -79  -152
 -13   -78    52
 -12   -77    43
 -11   137  -192
 -10   -79    82
  -9   -83   162
  -8   -82    94
  -7   -82   -48
  -6   -83   -97
  -5   203  -216
  -4   138   149
  -3   139   171
  -2   -81     9
  -1   -83   -89

H=   14,  K=    6

   0  -102   -42
   1  -104   -45
   2  -100    57
   3  -102   169
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```
  L    FO    FC

   4  -103     2
   5   -98     4
   6   -99  -102
   7   -99   -69
 -10   -97  -105
  -9  -102   292
  -8  -101    65
  -7  -104  -192
  -6  -101   122
  -5  -104   -96
  -4  -106  -132
  -3  -106   231
  -2  -100   106
  -1  -106  -183

H=    1,  K=    7

   0   267  -266
   1   137  -152
   2   181  -188
   3   353   350
   4   207   173
   5   -68    34
   6   -69   -70
   7   362  -341
   8   240   223
   9   428   417
  10   -74    52
  11   -76   -35
  12   112    93
  13   327  -311
  14   214   170
  15   142   140
  16   -72    -8
  17   -71    -4
 -17   136  -132
 -16   -73    26
 -15   224  -241
 -14   254   251
 -13   352   360
 -12   178   176
 -11   119  -133
 -10   -75    81
  -9   263  -268
  -8   -74   118
  -7   687   678
  -6   255  -265
  -5   203  -199
  -4   -68  -111
  -3   -68   -81
  -2   223  -203
  -1   575   559

H=    3,  K=    7

   0   223  -206
   1   532  -507
   2   171   194
   3   406   374
   4   106   119
   5   -73   125
   6   -70   -62
   7   360  -359
   8   -73   -48
   9   297   255
  10   202  -265
  11   241  -239
  12   -76   -27
  13   196  -119
  14   211   189
  15   119    80
  16   -73  -118
 -17   300  -310
 -16   113   -99
 -15   -75    -6
 -14   -78   136
 -13   409   399
 -12   299  -309
 -11   471  -477
 -10   -76     9
```

```
  L    FO    FC

  -9   134  -134
  -8   118  -158
  -7   602   543
  -6   257  -260
  -5   405  -378
  -4   -69   -57
  -3   126   137
  -2   227   205
  -1   440   389

H=    5,  K=    7

   0   186  -171
   1   679  -641
   2   153   133
   3   532   495
   4   108   139
   5   -73   -13
   6   254  -254
   7   439  -391
   8   -75   -52
   9   477   424
  10   183  -169
  11   -76    18
  12   128   -79
  13   130   -73
  14   174   202
  15   143   142
 -16   -77  -121
 -15   135  -110
 -14   112   102
 -13   248   278
 -12   188  -203
 -11   628  -616
 -10   267   293
  -9   223   233
  -8   186   214
  -7   390   386
  -6   154   162
  -5   940  -910
  -4   359   346
  -3   346   335
  -2   565   557
  -1   195   196

H=    7,  K=    7

   0   350  -345
   1   697  -709
   2   -73   -77
   3   622   606
   4   -73   -34
   5   -74   -15
   6   -78  -146
   7   329  -311
   8   -77   106
   9   417   385
  10   154  -178
  11   -75    -9
  12   -76   -75
  13   -76   -60
  14   -73    85
 -16   -74    30
 -15   130  -114
 -14   -77    25
 -13   301   298
 -12   -75    -6
 -11   -76   -68
 -10   182   205
  -9   -78    59
  -8   121   122
  -7   -76    94
  -6   198  -216
  -5   431  -419
  -4   193   201
  -3   631   610
  -2   -74   -96
  -1   -73   -62

H=    9,  K=    7
```

```
  L    FO    FC

   0   130  -145
   1   -79  -176
   2   135   136
   3   487   535
   4   -78    92
   5   329  -365
   6   -77    82
   7   265  -338
   8   151   190
   9   300   333
  10   -77  -124
  11   125  -157
  12   -73   -73
 -14   -73   -77
 -13   -77    76
 -12   -76   -28
 -11   167  -155
 -10   -77   -93
  -9   -78    34
  -8   -78     0
  -7   -78    55
  -6   340  -347
  -5   124  -156
  -4   -78   157
  -3   239   260
  -2   -78   -13
  -1   333  -341

H=   11,  K=    7

   0   -80   -51
   1   -79   -28
   2   196   207
   3   180   197
   4   128  -115
   5   166  -206
   6   -77    96
   7   -77     2
   8   -75    86
   9   123   159
  10   -74   -96
 -12   -76   -41
 -11   -77   -68
 -10   -77    33
  -9   125   104
  -8   -76     7
  -7   -80   -64
  -6   133   -84
  -5   -78   -64
  -4   175   211
  -3   204   285
  -2   115   105
  -1   -79    -7

H=   13,  K=    7

   0   -88   -98
   1   -88    54
   2   -87    54
   3   -89   214
   4   -89  -174
   5   -88   -85
   6   -85    -2
  -9   135   260
  -8   -86   -50
  -7   159  -181
  -6   -87   -40
  -5   -85    52
  -4   144    -7
  -3   150   209
  -2   125    60
  -1   -90  -242

H=    0,  K=    8

   0   321  -285
   1   375  -341
   2   -71    38
   3   -74   -78
```

L	FO	FC
4	117	124
5	346	330
6	222	-205
7	679	-659
8	-76	-46
9	172	143
10	-75	-32
11	-75	3
12	-75	-20
13	261	-212
14	-73	6
15	224	204
H=	2, K=	8
0	138	-101
1	758	-741
2	209	194
3	168	163
4	369	390
5	359	343
6	-76	117
7	307	-309
8	158	158
9	328	319
10	-77	-21
11	-77	95
12	-77	39
13	255	-244
14	140	83
15	278	263
-15	-74	-33
-14	126	107
-13	179	175
-12	120	-100
-11	-76	18
-10	-78	37
-9	-78	-94
-8	230	-275
-7	425	415
-6	-75	-24
-5	472	-479
-4	169	162
-3	226	-218
-2	-73	53
-1	180	179
H=	4, K=	8
0	213	-208
1	382	-384
2	125	134
3	483	475
4	-74	-13
5	250	236
6	137	-111
7	172	-126
8	187	167
9	362	315
10	214	-177
11	-76	51
12	-76	7
13	220	-245
14	116	148
-15	-72	70
-14	-74	58
-13	146	136
-12	180	-190
-11	402	-409
-10	346	329
-9	141	169
-8	-79	-141
-7	-77	-54
-6	269	-251
-5	286	-264
-4	126	134
-3	-74	-16
-2	-72	6
-1	167	160

L	FO	FC
H=	6, K=	8
0	374	-363
1	445	-406
2	-75	-29
3	304	315
4	133	-70
5	141	-165
6	-78	-83
7	242	-232
8	123	150
9	341	329
10	225	-210
11	140	-166
12	-73	25
13	-73	-96
-14	-74	20
-13	-78	142
-12	-77	94
-11	331	-334
-10	-75	59
-9	226	235
-8	190	-190
-7	-77	63
-6	164	-191
-5	295	-265
-4	295	258
-3	486	512
-2	-76	-90
-1	-76	10
H=	8, K=	8
0	-78	40
1	273	-283
2	183	201
3	227	223
4	164	-198
5	317	-334
6	-77	28
7	135	-193
8	192	204
9	321	368
10	137	-211
11	178	-193
-13	-75	94
-12	-75	111
-11	-76	-73
-10	-76	-32
-9	-77	93
-8	209	227
-7	140	146
-6	-77	40
-5	159	-156
-4	-79	120
-3	407	417
-2	115	-79
-1	307	-316
H=	10, K=	8
0	-78	-12
1	-78	-75
2	-79	-90
3	223	277
4	113	-165
5	289	-306
6	196	248
7	-76	37
8	-75	76
-10	-74	8
-9	109	121
-8	-75	10
-7	-78	69
-6	164	-211
-5	221	-260
-4	-78	-40
-3	240	270
-2	153	206
-1	-78	-79

L	FO	FC
H=	12, K=	8
0	-81	-54
1	-80	-38
2	-77	36
3	131	221
4	-77	16
-6	-78	-15
-5	-78	-75
-4	-78	54
-3	112	185
-2	-80	59
-1	-76	5
H=	1, K=	9
0	206	-184
1	241	-269
2	-77	107
3	-76	-30
4	-78	72
5	181	151
6	-77	-58
7	133	-153
8	130	115
9	190	157
10	263	-261
11	-74	-21
12	-72	-41
-13	150	164
-12	-73	-72
-11	-75	2
-10	110	-131
-9	-74	-62
-8	-77	41
-7	368	341
-6	170	169
-5	307	-326
-4	-76	-2
-3	134	115
-2	510	495
-1	-79	60
H=	3, K=	9
0	254	-235
1	336	-333
2	326	-324
3	-77	49
4	170	159
5	185	171
6	122	-129
7	-80	-106
8	156	171
9	232	208
10	-75	-73
11	-74	20
12	123	107
-12	160	-139
-11	-74	62
-10	105	57
-9	-75	65
-8	114	-73
-7	189	153
-6	-79	-82
-5	186	-183
-4	-77	-64
-3	132	-132
-2	-78	-28
-1	330	329
H=	5, K=	9
0	-79	-56
1	250	-225
2	-76	-30
3	116	116
4	159	162
5	-77	17

L	FO	FC
6	-73	40
7	125	-89
8	161	161
9	126	110
10	-72	15
11	157	-134
-12	-72	63
-11	247	-223
-10	217	214
-9	-75	86
-8	143	-149
-7	-75	25
-6	324	-311
-5	-78	-59
-4	295	284
-3	114	100
-2	-76	-44
-1	132	195
H=	7, K=	9
0	-77	-30
1	133	-119
2	197	231
3	116	93
4	209	-245
5	-77	-73
6	-74	-15
7	164	-184
8	-73	-25
9	208	239
-10	-74	12
-9	107	87
-8	166	-160
-7	228	226
-6	-74	-44
-5	257	-248
-4	297	301
-3	141	94
-2	172	-151
-1	233	203
H=	9, K=	9
0	-75	75
1	180	-165
2	138	135
3	-77	75
4	307	-389
5	-73	-42
6	145	192
-8	-73	17
-7	-75	17
-6	-75	-23
-5	262	-316
-4	-76	40
-3	236	256
-2	-76	-11
-1	-77	55
H=	0, K=	10
0	427	-391
1	-77	-72
2	221	230
3	111	-79
4	-75	-71
5	256	260
6	133	-135
7	-74	94
8	130	94
9	-73	-15
H=	2, K=	10
0	248	-248
1	257	-229
2	164	147
3	-77	77
4	108	-48

```
  L    FO     FC      L    FO     FC      L    FO     FC      L    FO     FC

  5   -77     44     -1   191    179     -8   176    142      1   -76   -129
  6   216   -250                         -7   122     79      2   170    209
  7   190   -156    H=     4,  K=   10   -6   118   -141      3   129    118
  8   291    250                         -5   -78   -123      4   -74    -93
 -9   -71    -24      0   130   -118     -4   206    162      5   -72     -6
 -8   -76    128      1   229   -236     -3   -76     14     -6   258   -271
 -7   -75    129      2   -76     39     -2   -76    -85     -5   139   -126
 -6   -74    -18      3   -73   -104     -1   121    120     -4   128    147
 -5   287   -266      4   -76    -33                         -3   116    -50
 -4   140    112      5   -72    -47    H=     6,  K=   10   -2   -75   -103
 -3   167    144      6   126   -145
 -2   158    175      7   149   -151      0   -75    -14
```

FIGURE 16

INNER COORDINATION SPHERE OF [ZnDAPP)]$_2$

The atomic numbering scheme and thermal ellipsoids are shown. Primed atoms are related to unprimed atoms of the same designation by a two-fold axis perpendicular to the Zn-Zn' and N1-N1' vectors.

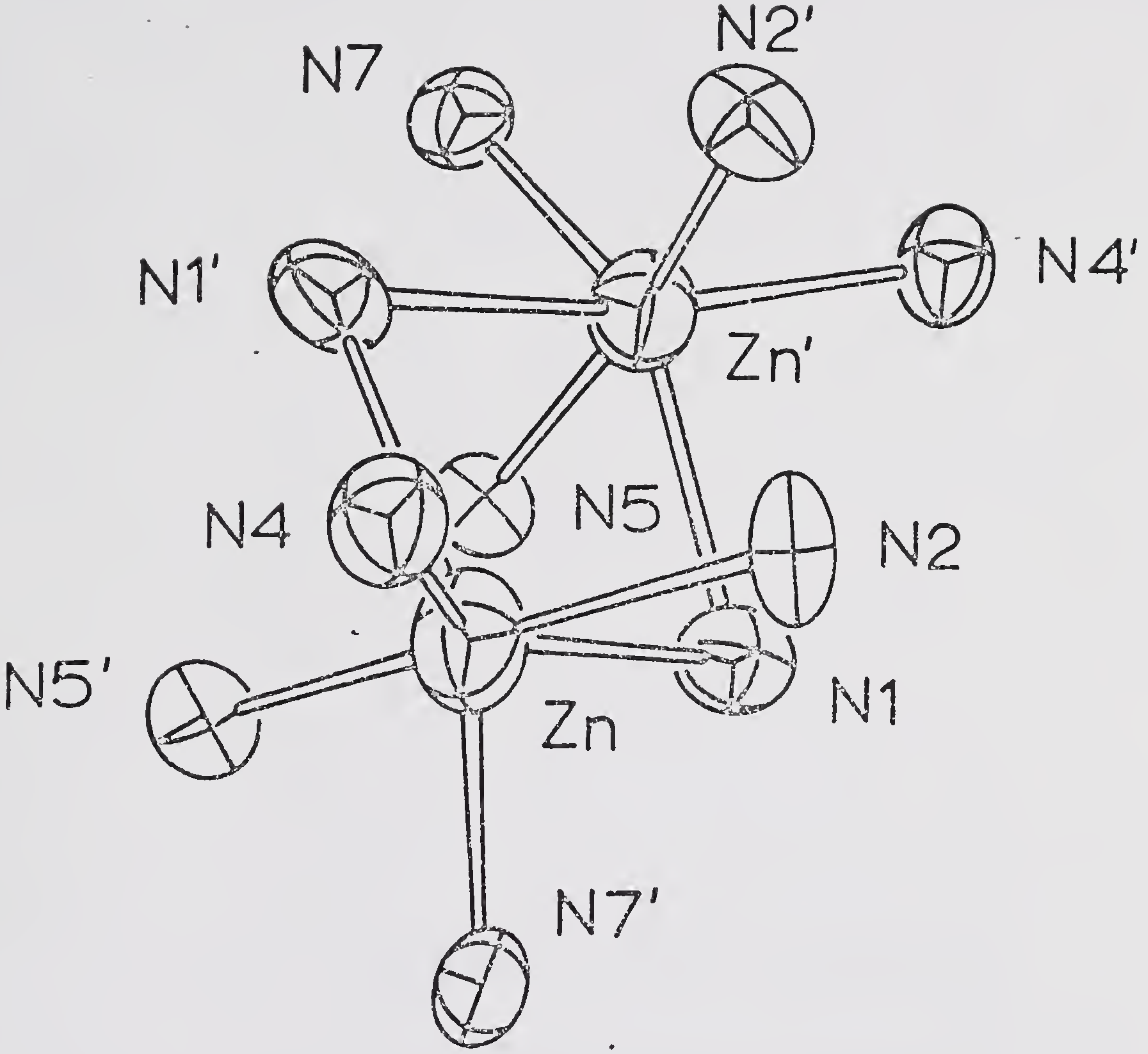

N7
N2'
N1'
N4'
Zn'
N4
N5
N2
N5'
N1
Zn
N7'

FIGURE 17

STEREOSCOPIC VIEW OF THE $[Zn(DAPP)]_2$ DIMER

The atomic numbering scheme is identical to that of Figure 10. Primed atoms are related to unprimed atoms of the same designation by a two-fold axis passing through the inner coordination sphere. Hydrogen atoms and some of the atomic labels are omitted for clarity.

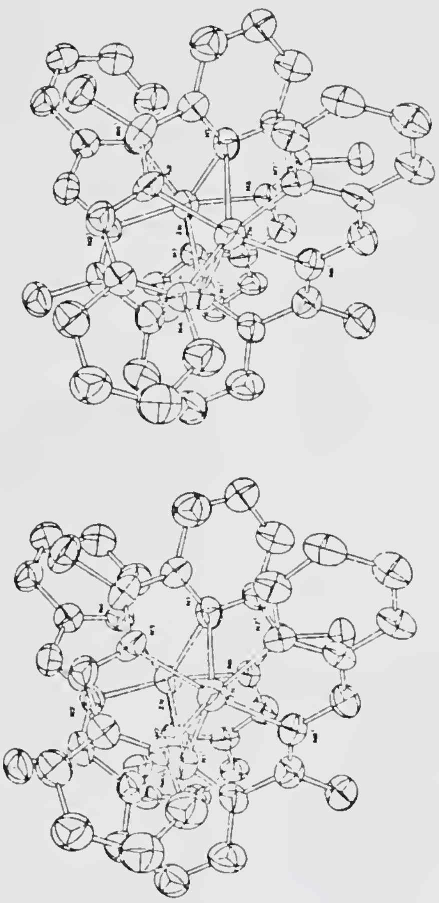
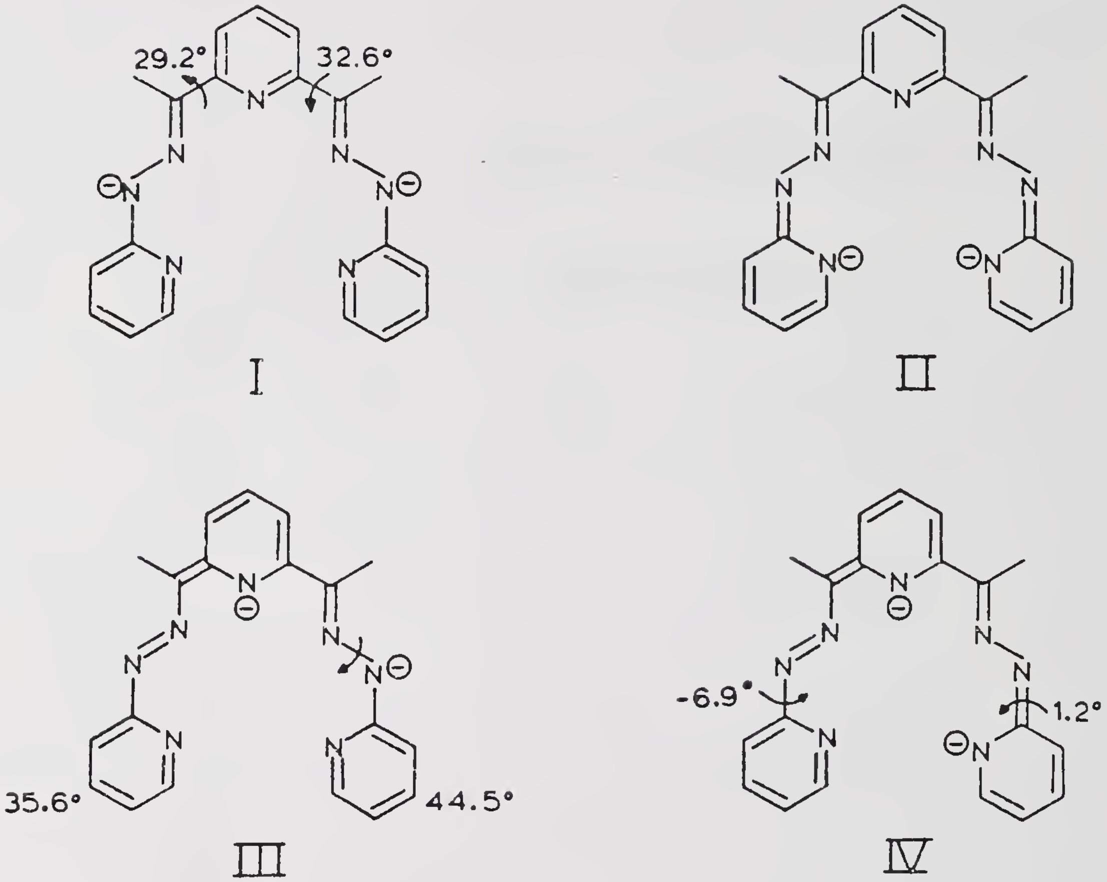


Table 46
TORSION ANGLES FOR Zn(DAPP)·$CHCl_3$·H_2O

DEFINING ATOMS	ANGLE
N1-C1-C6-N2	32.6
C2-C1-C6-C7	36.3
C7-C6-N2-N3	-0.9
C6-N2-N3-C8	8.4
N2-N3-C8-N4	1.2
N2-N3-C8-C9	0.2
N1-C5-C13-N5	29.2
C4-C5-C13-C14	34.9
C14-C13-N5-N6	-4.8
C13-N5-N6-C15	4.9
N5-N6-C15-N7	-6.9
N5-N6-C15-C16	-5.5
Zn-Zn'-N1'-N1	-9.8
Zn-Zn'-N1-N1'	9.0

simple covalency requirements and electrostatic and steric forces.[125] The zinc-nitrogen distances fall into two classes. The zinc-pyridylhydrazone nitrogen distances average 2.041(8) Å, similar to previously reported values.[66,67,117-120,126,127] The zinc-bridging pyridine nitrogen distances are considerably longer, Zn-N1 = 2.590(10)Å and Zn-N1' = 2.390(10)Å, and the difference of 0.2Å in these bonds results in an elongated Zn_2N_2 core. Such distortion has been observed in Zn-O clusters.[121,123] The angles of the central Zn_2N_2core are only slightly different from 90°, similar to a Zn_2N_2 core already identified.[128] The deviations of the core atoms from planarity are of the order of 0.1Å producing a torsion angle of -9.8° about the Zn'-N1' bond and 9.0° about the Zn'-N1 bond. The zinc-zinc distance of 3.503(2)Å is within the range of 3.03-3.55Å found for other clusters.[120-124,127]

The entire dimer is represented by the stereo view in Figure 17. Conjugation throughout the dianion DAPP does not produce a planar ligand as has been suggested.[23] Several resonance forms of DAPP are illustrated in Figure 18 and will be referred to in the following discussion. Torsion angles about the C1-C6 and C5-C13 bonds of 36.3° and 29.2°, respectively, produce a ligand highly distorted from the quasi-planar form of DAPPH. Three distinct planar portions (the two pyridylhydrazone residues and the central pyridine ring) are produced by the twisting about the C1-C6 and C5-C13 bonds. Resonance forms (I) and (II) of Figure 18



I

II

III

IV

FIGURE 18. RESONANCE FORMS FOR DAPP^{-2}.

The significance of the accompanying numbers is explained in the text.

contain single bonds at C1-C6 and C5-C13 and may be considered important in accounting for the twisting about these bonds. Resonance form (III) is useful in explaining the unequal tilt of the terminal pyridine rings with respect to the central ring. The pyridine ring containing N4 would be likely to rotate about the N3-N8 and N2-N3 bonds more than the ring containing N7 would be to rotate about the N6-C15 and N5-N6 bonds. The observed angles are 44.5° for the former and 35.6° for the latter. Resonance forms (III) and (IV) could be invoked to explain the tetrahedral geometry of N1 in this dimer. The formal negative charge on N1 results in two non-bonding electron pairs oriented in a suitable direction for bonding with the two zinc atoms. For DAPP, torsion angles of 1.2° and -6.9° are observed about the N3-C8 and N6-C15 bonds, respectively, while for DAPPH the corresponding angles are 12.0° and 10.0°. Resonance form (IV) places a double bond in one of these positions, explaining both the unequal amount of twisting and the smaller angles compared to DAPPH. The question which arises is why does the DAPP ligand twist since it is highly conjugated? Two explanations are offered. Since the pyridylhydrazones have been deprotonated and the resulting negative charges can be delocalized onto coordinated nitrogens (N1, N4, and N7), these nitrogens should have a tendency to form shorter bonds to the central metal ion due to coulombic attraction. However, as was observed in the case of DAPPH, the hydrogen-hydrogen interaction between the two terminal pyridine rings is significant and would be increased if these pyridine rings were drawn in closer. Thus the increased hydrogen-hydrogen interaction opposes the planarity induced by conjugation and forces the ligand to twist to such a degree and in such a manner that coordination to a single zinc becomes impossible and the ligand bridges two ions. In order to maintain a balanced charge distribution, a second ligand bridges the same two ions and the dimer results.

Another explanation is based on coulombic repulsion between the negatively charged pyridylhydrazones. These conjugated systems both carry negative charges and would repel each other. Since these systems are fairly rigid, twisting about the C1-C6 and C5-C13 bonds would be expected and is observed. Resonance form (II) is especially important here because the negative charges are placed on N4 and N7. These atoms would be very close together if the ligand were planar. A crystal structure determination of the zinc complex with the dianion derived from the Schiff base formed by condensation of o-aminobenzenethiol with 2,6-diacetylpyridine has been reported.[23] In this complex the ligand exhibits distortions intermediate between DAPP and DAPPH. This complex can be envisioned as an example in which the twisting of the ligand is not severe enough to preclude coordination to one metal ion. Although steric interactions among the methyl and adjacent hydrogens are proposed to cause the distortion from planarity in this case, interaction between the sulfur atoms could also be involved. This interaction could be of van der Waals or coulombic nature.

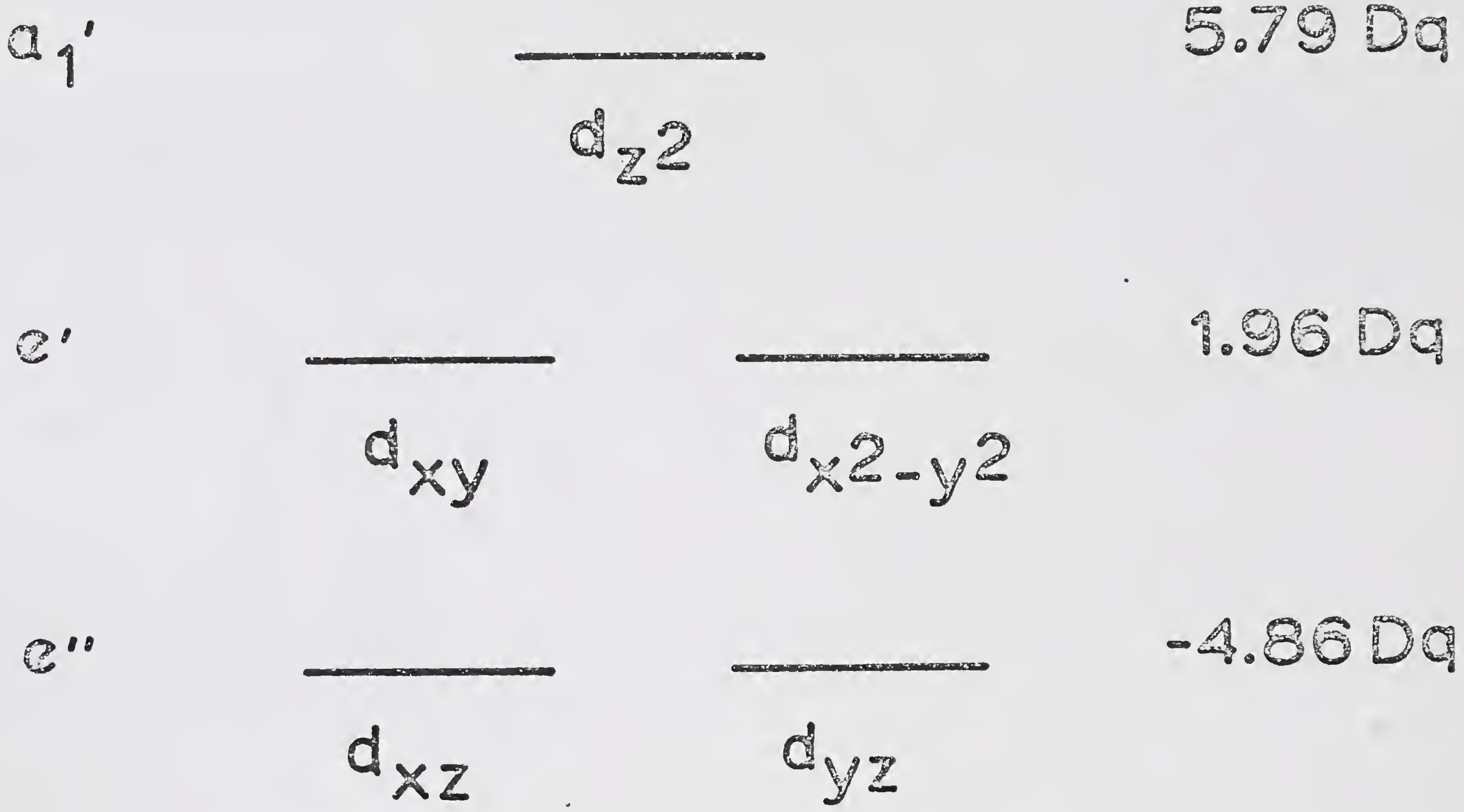
CHAPTER 7
GENERAL DISCUSSION

Seven-coordinated first-row transition metal complexes are currently of interest. The complexes and structures prepared and discussed in this work represent the first reported examples of seven-coordination for the Fe(II), Co (II), Ni(II), and Cu(II) ions. None of these ions have a spherically symmetric electron distribution and therefore CFSE is expected to be important. Although the reduced CFSE in a non-octahedral field has been employed as an argument against the formation of seven-coordinate complexes for these ions,[23,129,130] the results of this work indicate that the production of PB complexes may be only as difficult as the design and synthesis of ligands having sufficient constraints to produce this geometry.

The crystal field splitting for PB symmetry has been reported.[131,132] The energy level diagram is illustrated in Figure 19. The values of Dq for the levels are those of Spees _et_ _al_.[133] The PB geometry produces two orbitals, d_{xz} and d_{yz}, which are stabilized by -4.86Dq. The two orbitals directed at the ligands in the pentagonal plane, d_{xy} and $d_{x^2-y^2}$, are destabilized by 1.96Dq. The d_{z^2} orbital is directed at the two axial ligands and is destabilized by 5.79Dq. Table 47 lists the CFSE expected for octahedral and

FIGURE 19. CRYSTAL FIELD SPLITTING FOR PB (D_{5h}) GEOMETRY

The d orbital splittings in a PB crystal field are illustrated. Symmetry representation symbols are given on the left. The individual d orbitals in each group are listed in the center. The respective relative energy values in units of D_q are given on the right.


a1'
dz2
5.79 Dq
e'
dxy
dx2-y2
1.96 Dq
e''
dxz
dyz
-4.86 Dq

PB high spin complexes. The assumption has been made that the value of Dq does not change much upon going from hexacoordinated to heptacoordinated species.[133] The CFSE is slightly greater for the PB arrangement in the d^6 and d^7 cases, while the d^9 case favors octahedral geometry by only 0.20Dq. The largest discrepancy occurs for the d^8 case where the octahedral geometry is favored by 4.24Dq. Thus, the statement that seven-coordinate species have reduced CFSE as a result of non-octahedral geometry appears particularly applicable to the d^8 high spin case. However, the immediate assumption that replacement of an octahedral crystal field by a PB field result in reduced CFSE appears to be in question. Indeed, the stability of the $V(CN)_7^{-4}$ ion with respect to decomposition to $V(CN)_6^{-3}$ has been attributed to the CFSE gained by stabilizing two d orbitals relative to the others.[12]

Table 47
CFSE OF OCTAHEDRAL VS. PB GEOMETRY FOR HIGH SPIN CASES

# d electrons	5	6	7	8	9	10
Octahedral	0 Dq	-4.00	-8.00	-12.00	-6.00	0 Dq
PB	0 Dq	-4.86	-9.72	-7.76	-5.80	0 Dq

The design of ligands having sufficient constraints to produce PB complexes must take into account several factors. The steric interactions of the donor atoms appears to be less important than the interactions which may be present in the bulk of the ligand. For instance, DAPSC readily forms complexes as a planar pentadentate ligand whereas steric interactions between hydrogen atoms prohibit DAPPH from adopting a conformation equally as planar in its complexes. The role of steric interactions in other complexes with chelating ligands has been noted.[23,129] The electronic factors important to the proper design of ligands are primarily those involving conjugation effects in the ligand backbone. Pentadentate ligands containing planar backbones produced by conjugated systems are most likely to form PB complexes. However, the conjugation effects are not as straightforward as previously believed since the ligands suggested by Goedken and Christoph[23] to be planar due to conjugation effects have been shown to coordinate to Zn(II) in a non-planar manner. On the other hand, DAPP is expected to be extensively conjugated, but adopts a conformation much less planar than DAPPH. Obviously, the relative importance of steric/electronic effects is not readily apparent.

The structural studies in this work support the ordering of d orbital splittings in a PB field as suggested previously.[131-133] The trends observed in the metal-ligand distances are especially useful in illustrating this point. The d_{z^2} orbital is the only d orbital expected to interact strongly with the axial donors, while the d_{xy} and $d_{x^2-y^2}$ orbitals are expected to interact mainly with the planar pentagonal donor set. Thus, taking Mn(II) as a starting point, a decrease in the metal-donor bond lengths in the pentagonal plane is observed as electrons are added into the d_{xz} or d_{yz} orbitals, as in the [M(DAPSC)(H_2O)Cl]Cl·$2H_2O$ complexes where M=Fe(II) and Co(II). An increase in the metal-donor distances in the pentagonal plane is observed if the added electron enters the d_{xy} or $d_{x^2-y^2}$ orbital, as shown for the [Cu(DAPSC)(H_2O)$_2$]$^{++}$ cation relative to the isostructural Ni(II) cation. The trends exhibited by the metal-axial donor lengths are somewhat different than expected from electronic arguments alone. The apical donors seem to be more sensitive to the non-bonded contacts encountered than the electron configuration of the central metal ion present. The decreasing metal-axial donor distances observed as the central metal ion is varied from Mn(II) to Zn(II) correlates with the increasing metal-planar donor distances for the same series. In most cases the non-bonded contacts between the axial donors and planar donors in isostructural complexes are equivalent and suggest that the axial donor distances are greatly influenced by these contacts.

The deprotonation of metal complexes derived from ligands containing the 2-pyridylhydrazine residue has been studied recently.[114,134] Several of the deprotonated complexes containing Co(II) and Ni(II) had lowered magnetic moments. The complex prepared by Lions, Ni(DAPP), was reported to be dimagnetic.[129] The bridging deprotonated ligand DAPP in the dimeric [Zn(DAPP)]$_2$ structure suggests that a superexchange mechanism operating through bridging pyridine rings may be a factor in lowering the moments in

Co(II) and Ni(II) complexes. Superexchange through bridging ligands is well known, especially in the case of bridging oxygen atoms in Cu(II) complexes.[135-136]

A complex of DAPPH has been reported previously by Curry *et al*.[39] The complex was formulated as [Co(PyH)I]I (where PyH = DAPPH), a six-coordinate Co(II) complex. The conductivity of this complex in methanol was suggestive of a two-to-one electrolyte. In view of the PB structure of $[Co(DAPPH)(H_2O)_2]Cl_2$ and the planarity of DAPPH, some doubt is cast on the six-coordinate nature of [Co(PyH)I]I. The replacement of methanol for coordinated halide to produce a 2:1 electrolyte is consistent with formulation of the complex as either six- or seven-coordinate.

In conclusion, this work demonstrates that seven-coordinate first-row transition metal complexes may be more stable than was formerly assumed. The relative rarity of PB complexes may be due to synthetic difficulties rather than the intrinsic instability associated with non-octahedral complexes. The ligands used in this study consistently produce seven-coordinate species, and the number of ligands expected to produce PB complexes is limited only by the imagination of the researcher.

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I certify that I have read this study and that in my opinion it conforms to acceptable standards of scholarly presentation and is fully adequate, in scope and quality, as a dissertation for the degree of Doctor of Philosophy.

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